NBS MONOGRAPH 25 – SECTION 13

U.S. DEPARTMENT OF COMMERCE / National Bureau of Standards

Standard X-ray Diffraction Powder Patterns

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Section 13—Data for 58 Substances

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STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 13. --- Data for 58 Substances

by

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and

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Standard x-ray diffraction patterns are presented for 58 substances. Thirty-one of these patterns represent experimental data and 27 are calculated. The experimental x-ray powder diffraction patterns were obtained with an x-ray diffractometer. All d-values were assigned Miller indices determined by comparison with computed interplanar spacings consistent with space group extinctions. The densities and lattice constants were calculated and the refractive indices were measured whenever possible. The calculated x-ray powder diffraction patterns were computed from published crystal structure data. Both peak height and integrated intensities are reported for the calculated patterns.

Key words: Crystal structure; integrated intensities; lattice constants; peak intensities; powder patterns; reference intensities; standard; x-ray diffraction.

INTRODUCTION

The Powder Diffraction File is a continuing compilation of diffraction patterns gathered from many sources. Produced and published by the Joint Committee on Powder Diffraction Standards,[1] the File is used for identification of crystalline materials by matching d-spacings and diffraction intensity measurements. Under the partial sponsorship of the Joint Committee, the program at the National Bureau of Standards contributes new data to this File. Our work also aids in the evaluation and revision of published x-ray data and in the development of diffraction techniques. This report presents information for 58 compounds (31 experimental and 27 calculated patterns), and is the twenty-third of the series of "Standard X-ray Diffraction Powder Patterns."[2]

[1]Joint Committee on Powder Diffraction Standards, 1601 Park Lane, Swarthmore, PA. 19081. This Pennsylvania non-profit corporation functions in cooperation with the American Ceramic Society, the American Crystallographic Association, the American Society for Testing and Materials, The Clay Minerals Society, The Institute of Physics, the Mineralogical Association of Canada, the Mineralogical Society of America, The Mineralogical Society of Great Britain and Ireland, the National Association of Corrosion Engineers, and the Société Française de Minéralogie et de Cristallographie.

[2]See previous page for other published volumes.

EXPERIMENTAL POWDER PATTERNS

Sample. The samples used to make NBS patterns were obtained from a variety of sources or were prepared in small quantities in our laboratory. Appropriate annealing or recrystallization of the sample improved the quality of most of the patterns. A check of phase purity was provided by indexing the x-ray pattern. Unless otherwise noted, the spectrographic analyses were done at NBS after preparation of the sample was completed; the limit of detection for the alkali elements was 0.05 weight percent.

Optical data, color. A microscopic inspection for phase purity was also made on the non-opaque materials during the refractive index determination. The latter was done by grain-immersion methods in white light, using oils standardized in sodium light, in the refractive index range 1.40 to 2.1 [Hartshorne and Stuart, 1970].

The names of the sample colors were selected from the ISCC-NBS Centroid Color Charts [1965].

Interplanar spacings. For spacing determinations, a shallow holder was packed with a sample mixed with an internal standard (approximately 5 wt. percent tungsten powder). If tungsten lines were found to interfere with sample lines, silver or silicon was used in place of tungsten. If the internal standard correction varied along the length of the pattern, linear interpolations were used. To avoid errors associated with aberrations at the very top of peaks, the readings of 2θ were taken at positions about 20 percent of the way down from the top, and in the center of the peak width. The internal standard correction for each region was then applied to the measured value of 2θ. We have reported all data as $K\alpha_1$ peaks because the internal standard corrections for all regions were established in terms of the $K\alpha_1$ wavelength.

The internal standards used were of high purity (99.99%). The lattice constants used for them at 25 °C are given in the table below; the 2θ angles were computed using cell dimensions uncorrected for index of refraction.

Calculated 2θ Angles, $CuK\alpha_1$ λ = 1.540598Å

hkℓ	W a=3.16524Å ±.00004	Ag a=4.08651Å ±.00002	Si a=5.43088Å ±.00004
110	40.262		
111		38.112	28.443
200	58.251	44.295	
211	73.184		
220	86.996	64.437	47.303
310	100.632		
311		77.390	56.123
222	114.923	81.533	
321	131.171		
400	153.535	97.875	69.131
331		110.499	76.377
420		114.914	
422		134.871	88.032
511/333		156.737	94.954
440			106.710
531			114.094
620			127.547
533			136.897
444			158.638

The new internal standard Si powder is available as Standard Reference Material 640 [1974]. The lattice constant for the Si was refined from multiple powder data measurements made with tungsten as an internal standard [Swanson et al., 1966]. Cell parameter data were also collected for a single crystal from the boules ground to prepare the powder. The lattice parameters from the two methods agreed within 3 parts in 10^5 [Hubbard et al. 1975]. D-spacing results using SRM 640 will be in agreement with patterns recorded in this series of monographs since 1966.

All of our spacing measurements were recorded at 25 ± 1 °C on a diffractometer equipped with a focusing graphite or lithium fluoride crystal monochromator located between the sample and the scintillation counter. Pulse height discrimination was used as well. All measurements were performed using copper radiation: $\lambda(CuK\alpha_1, \text{peak})$= 1.540598Å [Deslattes and Henins, 1973].

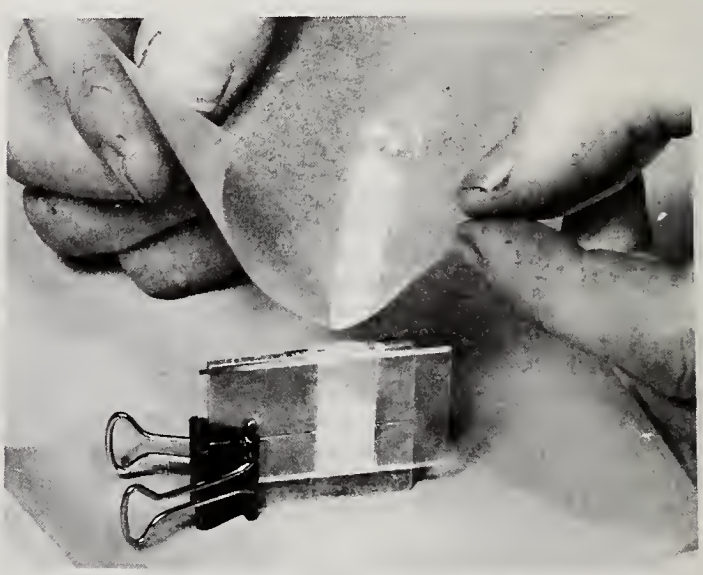
Structure, lattice constants. The space groups were listed with short Hermann-Maugin symbols as well as the space group numbers given in the *International Tables for X-ray Crystallography, Vol. I* [1952].

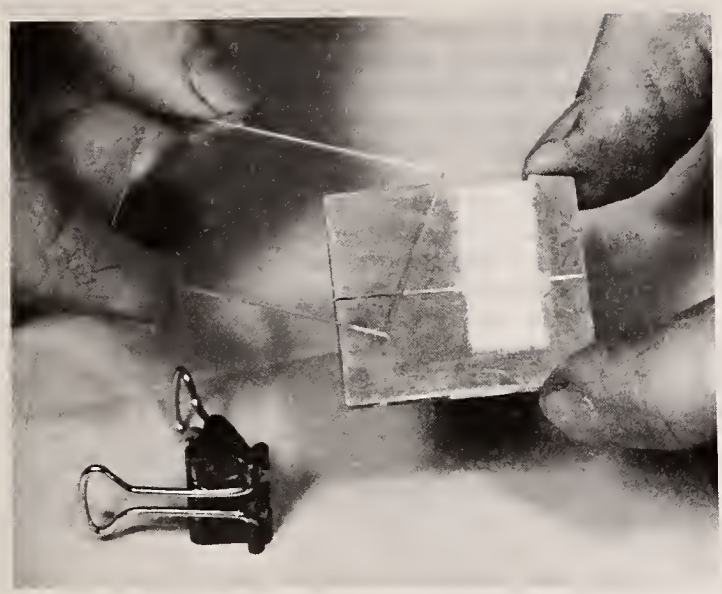
Orthorhombic cell dimensions were arranged according to the Dana convention b>a>c [Palache et al., 1944]. Monoclinic and triclinic lattice constants were transformed if necessary in order to follow the convention of *Crystal Data* [1973]. For primitive cells, the transformed cell axes are an alternate labelling of the reduced cell axes. For centered monoclinic cells, the transformed cell is the centered cell with the three shortest non-coplanar vectors.

A computer program [Evans et al., 1963] assigned hkℓ's and refined the lattice constants. Cell refinement was based only upon $2\theta_{obs}$ values which could be indexed without ambiguity. The program minimized the value $\Sigma(\theta_{obs}-\theta_{calc})^2$. The estimated standard deviations (e.s.d.'s) of the reciprocal cell parameters were determined from the inverse matrix of the normal equations. The program calculated the e.s.d.'s of the direct cell constants by the method of propagation of errors. Since 1973, the e.s.d.'s derived by the computer program have been increased by 50% in order to reflect more truly the uncertainty in the lattice constants. A similar increase should also be applied to all lattice constants in earlier publications of this series. In indexing cubic patterns, multiple hkℓ's were not utilized in the refinement or reported. Instead, the single appropriate index having the largest h was listed. The number of significant figures reported for d-values varied with the symmetry and crystallinity of each sample.

Densities. These were calculated from the specified lattice constants, the Avogadro number 6.0220943×10^{23} [Deslattes et al., 1974] and atomic weights based on carbon 12 [International Union, 1961].

Intensity measurements. It was found that samples which gave satisfactory intensity patterns usually had an average particle size smaller than 10 μm, as recommended by Alexander et al. [1948]. In order to avoid the orientation effects which occur when powdered samples are packed or pressed, a sample holder was made that had in its top face a rectangular cavity which extended to one end of the holder. To prepare the sample, a glass slide was clamped over the top face to form a temporary cavity wall (see Figure 1), and the powdered sample was allowed to drift into the end opening while the holder was held in a vertical





position. With the sample holder returned to a horizontal position, the glass slide was carefully removed so that the sample could be exposed to the x-ray beam (as shown in Figure 2). If the sample powder did not flow readily, or was prone to orient excessively, approximately 50 volume percent of finely ground silica-gel was added as a diluent. The intensities of the diffraction lines were measured as peak heights above background and were expressed in percentages of the strongest line. At least three patterns for intensity measurements were prepared for each sample to check reproducibility.

Reference Intensity Ratio, $I/I_{corundum}$. For reference intensity measurements, α-Al_2O_3 (corundum) was chosen as an internal standard to be mixed 1:1 by weight with the sample. This mixture of two components was mounted in our regular intensity sample holder (see Figures 1 & 2), and the pattern was taken. The reference intensity was then calculated as the direct ratio of the strongest line of the sample to the strongest line of corundum (hexagonal reflection (113)). In a few instances, the strongest line of one of the components coincided with a line of the other. In that case, the second strongest line was measured, and the value for the strongest line was then calculated.

CALCULATED POWDER PATTERNS

Since some substances of interest are not readily available for experimental work, powder patterns were calculated from published crystal structure data. The FORTRAN program used for the computations was developed by Clark, Smith and Johnson [1973] and modified at NBS.

Lattice parameters. Before the computations of the patterns, any necessary changes were made in the lattice constants in order to make them consistent with the revised value of $\lambda(CuK\alpha_1)$= 1.540598Å [Deslattes and Henins, 1973]. Both the altered and the original published values are given. Monoclinic and triclinic lattice constants were transformed if necessary, to follow the convention of *Crystal Data* [1973]. For primitive cells, the transformed cell axes are an alternate labelling of the reduced cell axes. For centered monoclinic cells, the transformed cell is the centered cell with the three shortest non-coplanar vectors.

Scattering factors. Whenever possible, the same scattering factors were used which the author of the reference article specified. Otherwise, the factors were taken directly from the *International Tables for X-ray Crystallography, Vol. III,* [1962]. The factors were corrected for dispersion if the author had done so.

Thermal parameters. The computer program used thermal parameter data of only two forms, the isotropic B's or the anisotropic β_{ij}'s in the following expressions:

$$e^{(-B \sin^2\theta)/\lambda^2}$$

or

$$e^{-(h^2\beta_{11}+k^2\beta_{22}+\ell^2\beta_{33}+2hk\beta_{12}+2h\ell\beta_{13}+2k\ell\beta_{23})}.$$

Other thermal parameters were converted to one of these two forms. The isotropic parameters were used directly, if given by the structure reference. In a few of our patterns, anisotropic parameters were also used directly as given by the structure reference; in other work, instead of using given anisotropic parameters, approximately equivalent isotropic values were substituted as defined by:

$$B = 4\left[\frac{\beta_{11}\beta_{22}\beta_{33}}{a^{*2}\, b^{*2}\, c^{*2}}\right]^{\frac{1}{3}}$$

Structural information. The atom positions used in these calculated patterns varied somewhat in the degree of reliability. When the expression "the structure was determined by..." was used, the atomic parameters in the reference cited had been calculated from refinement of single crystal data. When only the space group and structure type were given, the atomic positions had been derived by analogy with similar compounds whose structure was known. In cases where isostructural relationships were used, the atoms were in fixed special positions or the ionic radii were closely related to the corresponding radii of the atoms in the known structure.

Integrated intensities. The theoretical integrated intensity of reflection i on the "absolute/relative" scale is computed from the right hand side of the equation:

$$\frac{I_i^{abs}}{K} = \frac{M_i Lp_i |F_i T_i|^2}{2\mu V^2}$$

where:

F is the structure factor
T is the thermal correction

$Lp = \frac{1+\cos^2 2\theta}{\sin^2\theta\cos\theta}$ is the Lorentz-polarization term

M is the multiplicity for the reflection i
μ is the linear absorption coefficient
V is the volume of the unit cell

When the largest integrated intensity was assigned a relative value of 100 and all other reflections were scaled relative to it, the intensities were placed on the relative intensity scale (I^{rel}). Relative intensities were rounded to the nearest integer value before being listed, and reflections with I^{rel} less than 0.7 were omitted.

Scale factor (integrated intensities). The scale factor, γ, was defined to convert the tabulated I^{rel} to the "absolute/relative" scale [Hubbard, Evans and Smith]. That is:

$$\gamma = \frac{M'Lp'|F'T'|^2}{200\mu V^2}$$

and

$$\frac{I^{abs}}{K} = \gamma I^{rel}$$

The primes denoted the values for the largest integrated intensity. In earlier Monographs (1969-1975), a different scale factor, k_{NBS}, was reported which is related to γ:

$$\frac{\gamma}{k_{NBS}} = \frac{1}{2\mu V^2}$$

From γ, the theoretical value of the Reference Intensity Ratio, I/I_c, was calculated:

$$I/I_c = \frac{\mu\gamma\rho_c}{\mu_c\gamma_c\rho}$$

where ρ is the density and the subscript c represents corundum (α-Al_2O_3).

Peak intensities. The purpose of calculating peak intensities was to provide a tabulated pattern similar to what might be obtained from experimental diffractometer measurements. For each predicted reflection, Cauchy profiles centered at both the α_1 and the α_2 peak positions were calculated and summed, forming a simulated powder pattern. The full width at half-maximum (FWHM) was allowed to vary to represent the changing FWHM as a function of 2θ. [The values of the FWHM vs 2θ are given in the table below]. The resultant simulated powder pattern was then analyzed for peaks. In the regions of the predicted reflections several reflections could have identical or similar 2θ angles and produce only one composite peak in the simulated pattern. The 2θ angle of the composite peak was assigned the hkℓ of the reflection having the greatest contribution to the peak intensity. If any other peak contributed more than 10% of the intensity toward the composite peak intensity, a plus sign (+) was appended to the hkℓ. Peaks due solely to α_2 lines were omitted. If an α_1 peak and an α_2 peak overlapped, the α_1 reflection was listed only when it contributed a significant intensity (>10%) at the peak 2θ.

The peak search routine located peaks only at 2θ angles which were a multiple of 0.02°.

2θ CuKα_1	FWHM	2θ CuKα_1	FWHM
0°	0.12°	140	0.230
20	.12	145	.255
40	.12	150	.285
60	.125	155	.315
80	.130	160	.360
100	.135	162.5	.410
120	.155	165	.500
130	.185		

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Arsenic iodide, AsI_3

Sample
The sample was obtained from the City Chemical Company of New York.

Major impurities

0.001 to 0.01% each Bi, Sb
0.0001 to 0.001% each Fe, Si

Color
Bright orange

Structure
Hexagonal, $R\bar{3}(148)$, Z = 6 [Braekken, 1930].

NBS lattice constants of this sample:

a = 7.2093(8)Å
c = 21.449(3)

Density
(calculated) 4.702 g/cm^3

Reference intensity
$I/I_{corundum}$ = 1.3

Additional patterns
1. PDF card 7-272 [Swanson et al., 1956].
2. Hanawalt et al. [1938].
3. Heyworth [1931].

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CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
7.14	4	003	12.39
5.39	9	012	16.43
3.573	50	006	24.90
3.218	100	113	27.70
2.752	2	107	32.51
2.539	20	116	35.32
2.464	2	018	36.43
2.384	1	009	37.71
2.081	25	300	43.46
2.028	3	1·0·10	44.65
1.9882	20	119	45.59
1.8611	2	0·1·11	48.90
1.7982	16	306	50.73
1.7873	8	0·0·12	51.06
1.7680	2	0·2·10	51.66
1.7472	10	223	52.32
1.6097	5	226	57.18
1.6012	6	1·1·12	57.51
1.4378	4	229	64.79
1.4295	3	0·0·15,321	65.21
1.3560	4	3·0·12	69.23
1.3388	6	413	70.25
1.3291	5	1·1·15	70.84
1.2730	3	416	74.47
1.2693	3	2·2·12	74.73
1.1914	3	0·0·18,3·2·10	80.56
1.1825	4	419	81.30
1.0337	1	2·4·10	96.35

Barium silicate, β-$BaSiO_3$

Sample

The sample was prepared by repeated grindings and heatings at about 1100 °C of a 1:1 molar mixture of $Ba(OH)_2$ and silica gel.

Color

Colorless

Structure

Orthorhombic, Pmmm(47), Z=4, isostructural with $BaGeO_3$ and NH_4BeF_3 [Liebau, 1957; Toropov and Grebenshchikov, 1956].

NBS lattice constants of this sample:

a = 5.6182(5)Å
b = 12.445(1)
c = 4.5816(5)

Density

(calculated) 4.421 g/cm^3

Reference intensity

$I/I_{corundum}$ = 2.6

Polymorphism

Funk [1958] reports a second form below about 990°. Grebenshchikov et al. [1967] confirm this and report that the transformation is irreversible. They also suggest a third form (β').

Additional patterns

1. PDF card 6-247 [Levin and Ugrinic, 1953].
2. PDF card 12-651 [Funk, 1958].
3. PDF card 21-83 [Grebenshchikov et al.,1967].
4. Austin [1947].
5. Toropov and Grebenshchikov [1956].

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$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
6.23	2	020	14.20
5.12	14	110	17.30
4.174	11	120	21.27
3.693	35	021	24.08
3.552	15	101	25.05
3.418	100	111	26.05
3.339	65	130	26.68
3.112	55	040	28.66
2.808	25	200	31.84
2.740	10	210	32.65
2.723	10	140	32.86
2.699	14	131	33.17
2.574	8	041	34.82
2.353	17	211	38.22
2.342	11	141	38.41
2.325	4	230	38.69
2.293	17	002	39.26
2.235	25	221	40.32
2.186	2	051	41.26
2.123	<1	102	42.55
2.085	12	240	43.37
2.075	20	231,060	43.59
2.039	30	151	44.39
2.007	5	032	45.13
1.946	2	160	46.63
1.897	8	241	47.91
1.889	20	132,061	48.12
1.8629	4	250	48.85
1.8459	10	042	49.33
1.7932	6	320	50.88
1.7766	6	070,202	51.39
1.7588	5	212	51.95
1.7541	4	142	52.10
1.7337	7	301	52.76
1.7174	4	311	53.30
1.7067	5	330	53.66
1.6950	15	170	54.06
1.6685	2	260	54.99
1.6328	2	232	56.30
1.6151	1	152	56.97
1.6046	4	340	57.38
1.6002	4	331	57.55
1.5682	4	261	58.84
1.5554	1	080	59.37
1.5427	4	242	59.91
1.5387	4	062	60.08
1.5144	7	341	61.15
1.4989	2	180	61.85
1.4836	4	162	62.56
1.4734	6	081	63.04

d(Å)	I	hkℓ	2θ(°)
1.4649	4	113	63.45
1.4458	3	252	64.39
1.4350	3	123,033	64.93
1.4280	6	271	65.29
1.4247	3	181	65.46
1.4126	4	322	66.09
1.3958	4	410	66.99
1.3901	5	360,133	67.30
1.3690	3	332	68.48
1.3629	6	172	68.83
1.3490	1	262	69.64
1.3433	<1	401,203 +	69.98
1.3347	4	411,213	70.50
1.3304	5	430,361	70.76
1.3145	4	342	71.75
1.3126	4	421,223	71.87
1.3046	4	281	72.38
1.2886	4	191	73.42
1.2775	5	431,233	74.17
1.2688	3	153	74.76
1.2548	2	182	75.74
1.2444	2	0·10·0	76.49
1.2409	2	371,290	76.74
1.2304	2	063	77.52
1.2231	2	450	78.07
1.2009	1	0·10·1	79.80

Barium silicate (sanbornite), β-$BaSi_2O_5$

Sample
The sample was prepared by melting a 1:2 molar mixture of $BaCO_3$ and silica gel (at about 1430 °C) and annealing for 15 hours at 1325 °C. Because of the presence of a small amount of the high (α) form, the intensities are subject to a slight uncertainty.

Color
Colorless

Structure
Orthorhombic, Pmnb(62), Z=4. The structure has been determined by Douglass [1958].

NBS lattice constants of this sample:

a = 7.6922(8)Å
b = 13.525(1)
c = 4.6336(5)

Density
(calculated) 3.769 g/cm^3

Polymorphism
There is a high (α) form stable above 1350 °C [Roth and Levin, 1959]. This is given on PDF card 10-45 [Klasens et al., 1957].

Additional patterns
1. PDF card 10-46 [Klasens et al., 1957].
2. PDF card 11-170 (natural mineral)[Douglass, 1958].
3. Levin and Ugrinic [1953].
4. Oehlschlegel [1971].
5. Roth and Levin [1959].

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Roth, R.S. and Levin, E.M. (1959). J. Res. Nat. Bur. Stand. 62, 193.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
6.77	40	020	13.06
5.08	25	120	17.43
3.973	85	101	22.36
3.844	6	200	23.12
3.808	9	111	23.34
3.424	50	121	26.00
3.382	16	040	26.33
3.343	70	220	26.64
3.234	30	031	27.56
3.097	100	140	28.80
2.981	4	131	29.95
2.892	5	211	30.90
2.732	35	041	32.75
2.712	40	221	33.00
2.575	18	141	34.81
2.539	6	240	35.32
2.399	4	320	37.46
2.337	8	051	38.49
2.317	13	002	38.83
2.285	3	012	39.40
2.244	11	301	40.16
2.236	13	151	40.30
2.227	35	241	40.47
2.192	14	022	41.15
2.164	25	160	41.70
2.130	35	321	42.41
2.108	10	122	42.86
2.059	4	032	43.93
2.043	9	340	44.31
2.027	20	061	44.66
1.996	5	251	45.40
1.9907	8	132	45.53
1.9845	6	202	45.68
1.9233	9	400	47.22
1.9047	11	222	47.71
1.8693	3	341	48.67
1.8547	12	142	49.08
1.8501	10	420	49.21
1.8166	3	232	50.18
1.7932	19	261	50.88
1.7367	3	171	52.66
1.7114	5	242	53.50
1.7049	5	312	53.72
1.6918	16	080	54.17
1.6716	3	440	54.88
1.6663	3	322	55.07
1.6516	5	431,180	55.60
1.6175	3	271	56.88
1.6000	5	252	57.56
1.5881	6	081	58.03

d(Å)	I	hkℓ	2θ(°)
1.5812	10	162	58.31
1.5723	8	441	58.67
1.5552	6	181	59.38
1.5327	4	342	60.34
1.5144	2	103	61.15
1.5057	2	023,113	61.54
1.4840	5	451,072	62.54
1.4797	7	402	62.74
1.4676	8	281	63.32
1.4597	7	501	63.70
1.4508	4	511,352	64.14
1.4452	4	422	64.42
1.4352	2	133	64.92
1.4255	3	213	65.42
1.4115	4	380	66.15
1.4004	7	540	66.74
1.3953	8	461	67.02
1.3666	5	362,233	68.62
1.3555	3	442	69.26
1.3506	3	381	69.55
1.3443	4	182	69.92
1.3410	5	053,541	70.12
1.3319	2	1·10·0	70.67
1.3228	6	303	71.23
1.3196	5	243	71.43
1.2982	5	0·10·1,452	72.79
1.2801	8	1·10·1	73.99
1.2758	9	2·10·0,512	74.28
1.2696	5	480,333	74.71
1.2594	3	620,522	75.42
1.2328	3	532	77.34
1.2321	2	343	77.39
1.2244	3	481	77.97
1.2054	4	382	79.44

Barium silicate, Ba_2SiO_4

Sample
The sample was prepared by heating a 2:1 molar mixture of $BaCO_3$ and silicic acid at 1000 °C overnight, grinding and reheating at 1400 °C for 2 hours.

Color
Colorless

Structure
Orthorhombic, Pnam(62), Z=4, isostructural with α-K_2SO_4 [O'Daniel and Tscheischwili, 1942].

NBS lattice constants of this sample:

a = 7.508(1)Å
b = 10.214(1)
c = 5.8091(8)

Density
(calculated) 5.468 g/cm^3

Reference intensity
$I/I_{corundum}$ = 1.8

Additional patterns
1. PDF card 6-366 [Levin and Ugrinic, 1953].
2. Austin [1947].
3. Budnikov and Kulikova [1966].
4. Glushkova and Keler [1957].
5. Grebenshchikov et al. [1956].
6. O'Daniel and Tscheischwili [1942].
7. Shitova and Grebenshchikov [1972].
8. Toropov and Grebenshchikov [1956].

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CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
5.11	10	020	17.34
4.22	16	120	21.02
4.20	25	111	21.16
3.524	14	210	25.25
3.415	80	121	26.07
3.153	25	201	28.28
3.098	20	130	28.79
3.022	70	220	29.53
3.017	100	211	29.59
2.938	95	031	30.40
2.905	70	002	30.75
2.683	13	221	33.37
2.554	9	040	35.11
2.525	20	022	35.53
2.431	40	310	36.95
2.393	20	122	37.55
2.297	5	202	39.18
2.242	20	212	40.19
2.233	19	141	40.35
2.120	20	132	42.62
2.095	30	222	43.14
2.017	12	330	44.91
1.984	6	241	45.69
1.971	16	150	46.00
1.928	4	051	47.11
1.918	2	042	47.37
1.904	17	232	47.72
1.877	3	400	48.47
1.864	25	312	48.82
1.844	4	113	49.38
1.795	3	250	50.84
1.788	6	340	51.04
1.786	5	401	51.11
1.7594	25	411	51.93
1.7203	5	203	53.20
1.7084	35	341	53.60
1.6970	14	213	53.99
1.6832	14	033	54.47
1.6566	6	332	55.42
1.6438	6	430	55.89
1.6309	16	223	56.37
1.5967	5	161	57.69
1.5767	2	402	58.49
1.5507	4	260	59.57
1.5115	6	143	61.28
1.5066	6	422	61.50
1.4976	6	261	61.91
1.4684	4	062	63.28
1.4639	2	441	63.50
1.4524	9	004	64.06
1.4396	8	511	64.70
1.4301	7	432	65.18
1.4151	6	071	65.96
1.3822	2	450	67.74
1.3680	11	361	68.54
1.3479	3	403	69.71
1.3367	5	531	70.38

Barium silicate, $Ba_2Si_3O_8$

Sample
The sample was prepared by repeated grinding and heating at about 1400 °C of a 2:3 molar mixture of $BaCO_3$ and silica gel.

Color
Colorless

Structure
Monoclinic, $P2_1/a$ (14), Z = 4 [Kalscher and Liebau, 1965; Oehlschlegel, 1971]. $Ba_2Si_3O_8$ had earlier been reported with a similar cell with a/2 [Roth and Levin, 1959].

NBS lattice constants of this sample:

a = 13.960(3) Å
b = 4.6895(9)
c = 12.486(2)
β = 93.54(1)°

Density
(calculated) 3.964 g/cm^3

Reference intensity
$I/I_{corundum}$ = 1.8

Polymorphism
Oehlschlegel [1971] reports a reversible transformation of $Ba_2Si_3O_8$ at 1009 °C.

Additional patterns
1. PDF card 12-694 [Roth and Levin, 1959].
2. Austin [1947].

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CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
12.51	10	001	7.06
6.965	20	200	12.70
6.245	5	$\bar{2}01$	14.17
5.929	16	201	14.93
4.512	2	202	19.66
4.390	2	011	20.21
4.162	2	111,003	21.33
3.890	4	$\bar{2}10$	22.84
3.746	55	$\bar{2}11$,012	23.73
3.669	100	$\bar{2}03$	24.24
3.478	5	400,203	25.59
3.415	5	$\bar{4}01$	26.07
3.301	70	401,310	26.99
3.250	30	$\bar{2}12$	27.42
3.121	40	$\bar{4}02$	28.58
3.114	40	004	28.64
2.864	1	312	31.21
2.792	13	213	32.03
2.782	60	$\bar{2}04$	32.15
2.756	30	$\bar{4}11$,$\bar{4}03$	32.46
2.701	2	$\bar{4}11$	33.14
2.598	3	$\bar{4}12$	34.49
2.493	4	005	36.00
2.475	1	$\bar{2}14$	36.26
2.398	5	$\bar{4}04$,510	37.48
2.393	5	$\bar{2}05$,214	37.55
2.376	2	$\bar{5}11$,$\bar{4}13$	37.84
2.346	10	020	38.34
2.310	3	$\bar{6}01$	38.96
2.301	3	205	39.11
2.268	19	121,$\bar{4}13$	39.71
2.221	13	220,$\bar{6}02$	40.58
2.201	9	015	40.98
2.180	2	221	41.38
2.133	30	602,$\bar{2}15$ +	42.34
2.080	8	610,222	43.48
2.074	6	$\bar{3}21$	43.60
2.042	2	023	44.33
2.032	5	$\bar{3}15$,414	44.55
1.975	9	$\bar{2}23$,603	45.90
1.971	11	405	46.02
1.911	6	$\bar{4}21$	47.53
1.908	4	$\bar{4}15$	47.62
1.900	2	016	47.83
1.875	4	$\bar{4}22$,024	48.52
1.834	4	$\bar{4}06$	49.66
1.820	9	613	50.07
1.807	10	$\bar{2}16$	50.46
1.793	6	$\bar{3}16$,224	50.90
1.785	7	$\bar{7}12$,$\bar{4}23$	51.12

Barium silicate, $Ba_2Si_3O_8$ - continued

d(Å)	I	hkℓ	2θ(°)
1.780	19	007	51.28
1.776	13	$\bar{6}14,\bar{5}15$	51.42
1.753	6	$\bar{6}05$	52.12
1.751	6	$\bar{2}07$	52.20
1.738	5	423,406	52.63
1.705	2	$\bar{8}02,\bar{1}25$	53.73
1.649	8	620,605	55.69
1.645	5	$\bar{6}21$	55.85
1.631	4	$\bar{8}11$	56.36
1.628	6	416	56.46
1.612	3	$\bar{6}22,\bar{5}16$	57.09
1.608	3	811	57.26
1.598	3	217,$\bar{6}06$	57.65
1.578	1	622	58.45
1.556	2	$\bar{6}23,615$	59.34
1.550	4	031,$\bar{8}13$	59.59
1.515	2	032,$\bar{7}21$	61.10
1.508	2	425	61.42
1.500	5	208	61.79
1.476	2	232,$\bar{3}31$	62.93
1.4697	3	910,$\bar{9}11$ +	63.22
1.4636	1	$\bar{2}18,033$	63.51
1.4448	1	$\bar{4}26$	64.44
1.4208	3	$\bar{4}31$	65.66
1.4180	3	027,$\bar{1}27$	65.81
1.4038	2	127	66.56
1.3914	10	$\bar{6}17$	67.23
1.3485	3	625,$\bar{3}34$	69.67

Barium silicate, Ba_3SiO_5

Sample
The sample was prepared by repeated grindings and heatings at about 1400 °C of a 3:1 molar mixture of $BaCO_3$ and silica gel.

Color
Colorless

Structure
Tetragonal, I4/mcm (140), Z = 4, isostructural with Cs_3CoCl_5 and other similar compounds [Mansmann, 1965].

NBS lattice constants of this sample:

a = 7.3068(2)Å
c = 11.2275(6)

Density
(calculated) 5.763 g/cm^3

Reference Intensity
$I/I_{corundum}$ = 2.4

Polymorphism
Since Glushkova and Keler [1957] and Budnikov and Kulikova [1966] report patterns which differ considerably from the present study, the possibility of polymorphism cannot be ruled out.

Additional patterns
1. PDF card 19-175 [Budnikov and Kulikova, 1966].
2. PDF card 23-1027 [Brisi and Appendino, 1966].
3. Glushkova and Keler [1957].
4. Eysel [1970].

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CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
5.619	7	002	15.76
5.169	4	110	17.14
3.802	20	112	23.38
3.138	55	211	28.42
3.062	100	202	29.14
2.808	25	004	31.84
2.584	30	220	34.69
2.462	60	213	36.47
2.311	30	310	38.94
1.994	4	321	45.44
1.901	20	224	47.82
1.872	2	006	48.60
1.851	12	215	49.19
1.827	1	400	49.87
1.784	16	314	51.17
1.760	7	116	51.92
1.751	20	411	52.20
1.738	5	402	52.61
1.7224	2	330	53.13
1.6657	14	206	55.09
1.6465	16	332	55.79
1.6338	6	420	56.26
1.6018	16	413	57.49
1.5687	4	422	58.82
1.5311	3	404	60.41
1.5041	1	325	61.61
1.4676	1	334	63.32
1.4492	1	431	64.22
1.4402	4	217	64.67
1.4120	6	424	66.12
1.4034	3	008	66.58
1.3912	11	415	67.24
1.3881	10	512	67.41
1.3614	1	433	68.92
1.3473	1	521	69.74
1.3074	3	406	72.20
1.2917	2	440	73.22
1.2757	2	523	74.29
1.2677	6	336	74.84
1.2584	2	442	75.49
1.2534	5	530	75.84
1.2335	4	228	77.29
1.2307	3	426	77.50
1.2231	3	532	78.07
1.2179	4	600	78.47
1.1994	3	318	79.92
1.1944	3	611	80.32
1.1892	5	417	80.74
1.1737	1	444	82.04
1.1655	3	219	82.74

d(Å)	I	hkℓ	2θ(°)
1.1615	2	525	83.09
1.1442	8	534	84.63
1.1376	2	516	85.24
1.1350	2	541	85.48
1.1317	6	622	85.79
1.1172	5	604	87.18
1.1129	2	408	87.60
1.0916	1	543	89.77
1.0802	1	437	90.97
1.0732	3	2•0•10	91.74
1.0646	3	428	92.70
1.0591	2	615	93.32
1.0412	2	536	95.43
1.0335	1	710	96.38
1.0201	4	419	98.07
1.0174	3	545	98.42
1.0163	5	712	98.57
0.9997	2	721	100.80
.9972	4	642	101.15
.9830	5	626	103.19
.9742	1	2•1•11	104.51
.9695	3	554,723	105.22
.9615	2	617	106.48
.9565	1	4•0•10	107.28
.9530	2	644	107.85
.9504	1	448	108.29
.9457	2	732	109.09
.9405	2	3•3•10	109.97
.9347	6	538	111.00
.9298	1	547	111.88
.9252	<1	4•2•10	112.73
.9198	3	608	113.75
.9162	3	725	114.43
.9044	4	716	116.79
.9033	5	741	117.02
.9013	5	802,637	117.45
.8909	2	646	119.67
.8860	3	820	120.78
.8838	4	5•1•10	121.29
.8808	4	743	121.99

Barium silicate, $Ba_3Si_5O_{13}$

Sample
The sample was prepared by heating a 3:5 molar mixture of $BaCO_3$ and silica gel at about 1400°C with repeated grindings and reheatings. Because of problems related to orientation, the intensities are subject to some uncertainty.

Color
Colorless

Optical data
Biaxial(+), $N_\alpha = 1.612$, $N_\beta = 1.616$, $N_\gamma = 1.636$. 2V is about 35° [Oehlschlegel, 1971].

Structure
Monoclinic, $P2_1/c$ (14), Z = 4 [Roth, 1966; Oehlschlegel, 1971].

NBS lattice constants of this sample:

a = 20.208(3) Å
b = 4.7106(5)
c = 13.854(2)
β = 98.62(1)°

Density
(calculated) 3.874 g/cm^3

Additional patterns
1. PDF card 12-547 [Roth and Levin, 1959].
2. Oehlschlegel [1971].

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Roth, R. and Levin, E. M. (1959). J. Res. Nat. Bur. Stand. 62, 193.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
9.96	4	$2\bar{0}0$	8.87
6.80	16	$1\bar{0}2$	13.00
6.202	6	$\bar{1}02$	14.27
6.091	15	$\bar{2}02$	14.53
5.181	3	$\bar{3}02$	17.10
4.996	2	400	17.74
4.263	5	210	20.82
3.998	3	$21\bar{1}$,500	22.22
3.870	11	$\bar{1}12$	22.96
3.844	55	310	23.12
3.773	100	$\bar{4}02$	23.56
3.729	10	$\bar{2}12$	23.84
3.622	2	$\bar{3}11$	24.56
3.484	3	$\bar{3}12$	25.55
3.424	7	410,004	26.00
3.328	20	$\bar{6}00$	26.77
3.249	85	$\bar{3}0\bar{4}$,411 +	27.43
3.199	40	$\bar{4}12$	27.87
3.100	20	$20\bar{4}$	28.78
3.045	2	510,$\bar{4}04$	29.31
2.909	6	$\bar{5}12$	30.71
2.875	13	304	31.08
2.855	5	$\bar{7}00$	31.31
2.788	75	$\bar{1}14$,$\bar{7}02$	32.08
2.769	25	014	32.30
2.718	2	610	32.93
2.698	3	114	33.18
2.644	3	404	33.87
2.607	2	$61\bar{1}$	34.37
2.589	2	214,$\bar{6}04$	34.62
2.558	1	$\bar{4}14$	35.05
2.497	1	$\bar{8}00$	35.93
2.469	3	$\bar{8}02$	36.36
2.443	2	710	36.76
2.429	4	612,504	36.98
2.356	14	020	38.17
2.283	6	$00\bar{6}$	39.44
2.273	25	$\bar{2}21$	39.61
2.269	13	$\bar{6}14$	39.69
2.241	5	802,215	40.21
2.230	18	$\bar{1}06$	40.41
2.224	15	$\bar{1}22$,$\bar{8}11$	40.53
2.211	35	712,$\bar{9}02$	40.77
2.206	30	810,$\bar{4}06$	40.87
2.175	4	321	41.49
2.158	9	514,$\bar{2}06$	41.82
2.124	5	$\bar{4}21$,$\bar{5}06$	42.53
2.068	11	$\bar{2}16$,123 +	43.73
2.043	3	$\bar{3}16$	44.31
2.025	7	902,812	44.72
2.008	8	$\bar{9}10$	45.11
2.004	16	$\bar{9}04$	45.20
1.999	15	422,10·0·0 +	45.33
1.980	2	$\bar{4}23$	45.79
1.923	2	620	47.22

Barium silicate, $Ba_3Si_5O_{13}$ - continued

d(Å)	I	hkℓ	2θ(°)
1.908	8	$\bar{5}23,\bar{3}24$	47.61
1.888	5	804	48.15
1.8755	4	$\underline{\quad}224$	48.50
1.8504	4	$\overline{10}\cdot0\cdot\underline{4}$	49.20
1.8445	12	$10\cdot0\cdot2,\bar{9}14$	49.37
1.8410	15	$\overline{10}\cdot\underline{1}\cdot2,10\cdot1\cdot0$	49.47
1.8223	8	$\bar{1}17,324$ +	50.01
1.8162	35	$11\cdot0\cdot0,416$ +	50.19
1.7988	8	$\bar{7}22$	50.71
1.7854	11	$025,\bar{7}16$	51.12
1.7635	4	$\underline{1}25,606$	51.80
1.7276	6	$\bar{1}08,\bar{9}06$	52.96
1.7040	2	$\bar{8}22,\bar{8}16$	53.75
1.6657	2	$706,12\cdot0\cdot0$ +	55.09
1.6386	3	026,914	56.08
1.6296	12	$10\cdot\underline{1}\cdot3,\overline{10}\cdot0\cdot6$	56.42
1.6253	8	$\bar{9}\underline{2}1,\bar{2}18$ +	56.58
1.6209	8	$\bar{9}16$	56.75
1.6167	8	$\bar{3}\underline{1}8,\underline{8}15$ +	56.91
1.6118	7	$\bar{9}22,\underline{11}\cdot1\cdot4$	57.10
1.5984	3	$\bar{4}18$	57.62
1.5782	2	$\bar{9}23,\bar{5}26$	58.43
1.5547	6	$\underline{2}18$	59.40
1.5509	9	$230,\underline{13}\cdot0\cdot2$	59.56
1.5360	2	$\bar{6}18,922$	60.20
1.5284	4	330	60.53
1.5141	2	$\bar{2}27,\bar{1}27$ +	61.16
1.5103	1	$\underline{12}\cdot1\cdot\underline{4},426$	61.33
1.4948	2	$508,\bar{7}18$ +	62.04
1.4859	4	$\bar{1}33,12\cdot1\cdot2$	62.45
1.4770	2	$\bar{4}32$	62.87
1.4732	2	$\underline{9}23,824$ +	63.05
1.4616	3	$\bar{5}31,530$ +	63.61
1.4526	2	$\overline{12}\cdot0\cdot6,10\cdot2\cdot2$ +	64.05
1.4498	2	432	64.19
1.4418	7	$\overline{11}\cdot2\cdot2,\overline{14}\cdot0\cdot2$	64.59
1.4386	7	$11\cdot2\cdot0,10\cdot1\cdot5$	64.75
1.4272	2	$034,14\cdot0\cdot0$	65.33
1.4155	4	$12\cdot0\cdot4,916$ +	65.94
1.4117	4	626	66.14
1.4003	3	$\underline{\quad}\bar{9}18,\bar{7}\underline{2}7$	66.75
1.3936	8	$\underline{14}\cdot0\cdot\underline{4},\bar{1}28$	67.11
1.3852	2	$\bar{2}\cdot\underline{0}\cdot10,028$	67.57
1.3782	2	$\bar{4}\underline{2}8,334$	67.96
1.3662	4	$\bar{1}35,\underline{12}\cdot2\cdot2$ +	68.64
1.3583	1	$11\cdot1\cdot5,527$	69.10

Cadmium silicate, Cd_2SiO_4

Sample
The sample was prepared by heating at 1200 °C, for several hours, a 2:1 molar mixture of CdO and silica gel. The sample was ground and reheated several times at 1000 °C for one hour each time. A small amount of Cd_3SiO_5 was present and this may slightly distort the intensity measurements.

Color
Colorless

Structure
Orthorhombic, Fddd(70), Z=8. Isostructural with Na_2SO_4(V). The structure was studied by Glasser and Glasser [1964].

NBS lattice constants of this sample:

a = 9.805(1)Å
b = 11.807(2)
c = 6.013(1)

Density
(calculated) 6.047 g/cm^3

Reference intensity
$I/I_{corundum}$ = 2.1

Additional pattern
1. PDF card 17-258 [Glasser and Glasser, 1964].

References
Glasser, L.S.D. and Glasser, F.P. (1964). Inorg. Chem. 3, 1228.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
4.704	15	111	18.85
3.770	45	220	23.58
2.951	65	040	30.26
2.790	100	311	32.06
2.678	90	022	33.43
2.563	25	202	34.98
2.449	3	400	36.66
2.352	6	222	38.24
2.320	35	331	38.78
2.145	8	151	42.10
1.936	20	113,242	46.90
1.841	20	511	49.48
1.824	35	260,351	49.97
1.758	3	133	51.99
1.691	20	313	54.19
1.685	13	531	54.39
1.647	20	062	55.78
1.603	2	171	57.45
1.575	7	620	58.55
1.567	14	333	58.88
1.504	5	004	61.63
1.476	4	080	62.91
1.454	10	371	63.96
1.436	6	602	64.90
1.396	5	224	66.97
1.393	5	513	67.17
1.3843	6	353	67.62
1.3396	8	044	70.20
1.3199	2	533	71.41
1.2909	5	642	73.27
1.2789	3	282	74.07
1.2571	3	660	75.58
1.2259	1	800	77.86
1.2052	3	553	79.46
1.2003	4	373	79.85
1.1932	3	391	80.42

Cadmium silicate, Cd_3SiO_5

Sample

The sample was made by heating a 3:1 molar mixture of CdO and silica gel at 1100 °C for 2 hours. The product was then ground and reheated at 700 °C for 20 hours. The sample showed some hydration products after standing in air and also contained a very slight percentage of Cd_2SiO_4; therefore, the intensities may be slightly in error.

Color

Greenish yellow.

Structure

Tetragonal, P4/nmm (129), Z = 2 [Eysel, 1970]. Eysel (1970) suggested also a possible monoclinic cell. The broadening of some lines in patterns from this sample indicates that it probably is of lower symmetry.

NBS lattice constants of this sample:

a = 6.842(2)Å
c = 4.952(2)

Density

(calculated) 6.379 g/cm^3

Reference intensity

$I/I_{corundum}$ = 5.4

Additional patterns

1. PDF card 17-257 [Dent Glasser and Glasser, 1964].
2. Eysel [1970].

References

Dent Glasser, L. S. and Glasser, F. P. (1964). Inorg. Chem. 3, 1228.

Eysel, W. (1970). Neues Jahrb. Mineral. Monatsh. 1970, 534.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
4.96	5	001	17.88
4.85	8	110	18.29
4.015	3	101	22.12
3.462	5	111	25.71
3.420	2	200	26.03
2.814	100	201	31.77
2.604	<1	211	34.41
2.476	11	002	36.25
2.419	20	220	37.14
2.327	4	102	38.66
2.206	3	112	40.88
2.173	5	221	41.53
2.165	5	310	41.68
2.071	2	301	43.68
2.006	3	202	45.16
1.982	3	311	45.70
1.924	1	212	47.20
1.730	20	222	52.87
1.710	10	400	53.55
1.677	1	302	54.68
1.629	1	312	56.44
1.616	1	401	56.94
1.613	2	330	57.04
1.562	1	113	59.08
1.530	1	420	60.44
1.5066	1	322	61.50
1.4861	7	203	62.44
1.4616	14	421	63.61
1.4072	6	402	66.38
1.3782	1	412	67.96

Calcium hydrogen phosphate hydrate, $Ca_8H_2(PO_4)_6 \cdot 5H_2O$

Sample
The sample was obtained from B. Dickens at NBS. Brown et al. [1962] prepared the sample. The intensity of the strongest line was very high compared to the other reflections. Therefore, the intensity of the second strongest line (d=2.833) was assigned the value of 100 and all other reflections were scaled to it. On that scale the strongest line at d=18.67 has I ≈300.

Color
Colorless

Optical data
Biaxial(-), N_α = 1.576, N_β = 1.583, N_γ = 1.585. 2V is ≈50° [Brown et al, 1962].

Structure
Triclinic, Z = 2. The structure was determined by Brown et al.[1962] and refined by Dickens et al. [1973].

NBS lattice constants of this sample:

a = 9.529(3) Å
b = 18.994(4)
c = 6.855(3)
α = 92.33(3)°
β = 90.13(3)
γ = 79.93(2)

Density
(calculated) 2.673 g/cm^3.

Reference intensity
$I/I_{corundum}$ = 0.5. This measurement is based on the line at 2.833A (designated as 100).

Additional patterns
1. PDF card 11-184 [Bjerrum, 1958].
2. PDF card 13-391 [Hayek et al, 1960].
3. Lehr et al. [1967].

References

Bjerrum, N. (1958). Kgl. Dan. Vidensk. Selsk. Mat. Fys. Medd. 31, Nr. 7, 22.

Brown, W.E., Smith, J.P., Lehr, J.R.,and Frazier, A. W. (1962). Nature (London) 196, 1050.

Dickens, B., Schroeder, L. W., and Brown, W. E. (1973). Am. Crys. Assoc. (Abs.-Winter Meeting) B2, 26.

Hayek, E., Newesely, H., Hassenteufel, W., and Krismer, B. (1960). Monatsh. Chem. 91, 249.

Lehr, J. R., Brown, E. H., Frazier, A. W., Smith, J.P., and Thrasher, R.D.(1967).Tenn. Val. Auth. (Chem. Eng. Bull.) No. 6.

CuKα$_1$, λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
18.67	300	010	4.73
9.36	45	100,020	9.44
9.05	40	$1\bar{1}0$	9.77
6.10	6	$\bar{1}20$	14.51
5.52	25	$\bar{1}01$	16.04
5.417	7	111,021	16.35
5.211	4	$1\bar{1}1$	17.00
5.101	12	$\bar{1}11$	17.37
4.815	6	$\bar{1}30$	18.41
4.706	5	$03\bar{1}$	18.84
4.670	4	040	18.99
4.514	10	$03\bar{1}$,140 +	19.65
4.492	10	$\bar{1}21$	19.75
4.294	7	131	20.67
4.111	5	230	21.60
3.919	16	$\bar{2}20$,$\bar{1}40$ +	22.67
3.879	12	201,$\bar{1}31$	22.91
3.862	10	$\bar{2}01$	23.01
3.786	10	041	23.48
3.745	14	221	23.74
3.660	30	$\bar{2}11$	24.30
3.492	25	$23\bar{1}$	25.49
3.441	50	$22\bar{1}$	25.87
3.424	60	002	26.00
3.378	18	$\bar{2}21$	26.36
3.311	20	$\bar{1}\bar{5}1$	26.91
3.278	18	$\bar{1}50$	27.18
3.209	25	$\bar{1}02$,250 +	27.78
3.180	25	241,310	28.04
3.132	10	$\bar{1}\bar{2}2$,300 +	28.48
3.117	7	$\bar{1}12$,060	28.62
3.055	14	$03\bar{2}$,$2\bar{4}0$	29.21
3.015	8	330	29.61
2.946	14	$\bar{1}22$,$\bar{2}\bar{5}1$	30.31
2.914	12	$\bar{1}51$	30.66
2.873	30	251	31.10
2.833	100	260	31.55
2.820	95	$\bar{3}20$,$24\bar{1}$	31.70
2.779	45	$\bar{1}\bar{4}2$,$33\bar{1}$	32.18
2.745	35	$\bar{1}32$,331	32.59
2.707	25	222,042	33.06
2.671	50	070	33.53
2.637	35	$16\bar{1}$,350	33.97
2.617	20	$\bar{3}30$	34.23
2.606	20	$2\bar{2}2$,341	34.38
2.567	16	$\bar{1}61$,$\bar{1}\bar{5}2$	34.93
2.544	12	$\bar{1}71$,$2\bar{5}1$	35.25
2.486	5	$\bar{2}51$	36.10
2.475	8	$05\bar{2}$,171	36.27
2.458	5	$\bar{1}70$	36.52

Calcium hydrogen phosphate hydrate, $Ca_8H_2(PO_4)_6 \cdot 5H_2O$ - continued

d(Å)	I	hkℓ	2θ(°)
2.365	7	180	38.01
2.335	8	080,$\bar{2}$71 +	38.52
2.304	7	252,$\bar{3}$02 +	39.06
2.271	5	$\bar{3}$61,3$\bar{1}$2	39.66
2.265	6	$\bar{1}\bar{8}$1,162	39.77
2.258	7	062,$\bar{3}\bar{4}$1	39.89
2.215	16	1$\bar{6}$2,$\bar{3}$50	40.71
2.158	5	$\bar{3}$22,$\bar{4}\bar{4}$1	41.83
2.136	7	441	42.27
2.106	9	190	42.90
2.088	7	$\bar{2}$52	43.29
2.063	6	$\bar{2}\bar{7}$2,$\bar{2}\bar{1}$3 +	43.85
2.036	5	$\bar{1}$33,$\bar{3}$60 +	44.46
2.002	8	2$\bar{6}$2	45.25
1.998	9	4$\bar{3}$1	45.35
1.990	10	191	45.55
1.957	7	$\bar{4}\bar{2}$2,$\bar{1}$90	46.36
1.948	17	$\bar{3}$42,381 +	46.58
1.936	18	$\bar{3}$61	46.88
1.929	11	291,2$\bar{3}$3	47.06
1.914	11	053	47.46
1.897	10	1·10·0,$\bar{3}\bar{7}$2 +	47.92
1.891	10	530	48.07
1.848	20	303,$\bar{1}$·$\bar{1}$0·1	49.27
1.837	20	$\bar{3}$52,3$\bar{9}$1 +	49.59
1.832	18	253,5$\bar{1}$1 +	49.72
1.804	15	391,$\bar{2}$·$\bar{1}\bar{0}$·1	50.54
1.745	8	2$\bar{9}$1,462	52.39
1.743	8	551	52.47
1.725	10	1·11·0	53.05
1.710	25	490	53.55

Cobalt phosphate, $Co(PO_3)_2$

Sample
The sample was prepared by heating a 1:2 molar mixture of $CoCO_3$ and H_3PO_4 to about 640 °C for 15 hours.

Color
Deep purplish red.

Structure
Monoclinic, I2/a(15) or Ia(9), Z = 8 [Beucher and Grenier, 1968]. These authors gave the cell in the settings C2/c(15) or Cc(9).

NBS lattice constants of this sample:

a = 11.189(3)Å
b = 8.287(2)
c = 9.926(4)
β = 112.42(3)°

Density
(calculated) 3.386 g/cm^3

Reference intensity
$I/I_{corundum}$ = 1.4

Additional pattern
1. PDF card 19-351 (Sarver, 1966).

References
Beucher, M. and Grenier, J.-C. (1968). Mater. Res. Bull. 3, 643.
Sarver, J.F. (1966). Trans. Brit. Ceram. Soc. 65, 191.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
6.45	6	110	13.71
6.146	40	011	14.40
4.576	20	$\bar{2}11$	19.38
4.251	35	$\bar{1}12$	20.88
3.742	6	$\bar{1}21$	23.76
3.538	20	211	25.15
3.378	30	112,121	26.36
3.232	12	220	27.58
3.184	30	$\bar{3}10$	28.00
3.001	100	$\bar{2}22$	29.75
2.868	20	013	31.16
2.670	3	$\bar{1}30$	33.54
2.635	4	$\bar{4}11$	34.00
2.586	20	400	34.66
2.466	4	$\bar{2}31$	36.40
2.389	20	$\bar{2}22$	37.62
2.378	9	$\bar{3}23$	37.80
2.279	6	$\bar{3}14$	39.51
2.193	7	420,411	41.13
2.177	7	$\bar{4}04$	41.45
2.156	3	330,$\bar{5}12$	41.86
2.099	20	$\bar{2}33$	43.07
2.071	4	040	43.68
2.016	8	114,$\bar{1}41$	44.93
1.956	6	402	46.38
1.928	4	$\bar{4}24$	47.10
1.895	2	$\bar{5}23$	47.96
1.872	3	$\bar{2}42$	48.61
1.854	3	$\bar{4}33$	49.10
1.824	2	$\bar{4}15$	49.97
1.799	5	$\bar{3}34$	50.71
1.757	8	233	52.00
1.754	6	431,$\bar{1}43$	52.09
1.735	6	$\bar{5}32$	52.70
1.701	7	$\bar{6}22$	53.85
1.6314	10	051,512	56.35
1.6167	7	440	56.91
1.6115	7	$\bar{2}35$,314	57.11
1.5376	6	044	60.13
1.5295	6	006	60.48
1.5250	7	$\bar{6}33$	60.68
1.5009	4	$\bar{4}44$	61.76

Copper imidazole nitrate, $Cu(C_3H_4N_2)_4(NO_3)_2$

Sample

The sample was prepared at NBS by C. W. Reimann by evaporating an aqueous solution of $Cu(NO_3)_2$ and imidazole ($C_3H_4N_2$) at room temperature. It was difficult to obtain intensities because the sample deteriorated somewhat when exposed to x-rays.

Color

Unground: deep blue

Optical Data

Biaxial (-), N_α =1.584, N_β = 1.610, N_γ = 1.645. 2V ≈ 40°. The sample shows pleochroism.

Structure

Orthorhombic, Pmnb(62), Z=4, [Mighell, Santoro, and Reimann, private comm.].

NBS lattice constants of this sample:

a = 13.396(3)Å
b = 13.858(3)
c = 9.825(2)

Density

(calculated) 1.675 g/cm^3

Reference intensity

$I/I_{corundum}$ = 1.0

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
8.01	8	011	11.04
6.87	19	111	12.87
6.697	6	200	13.21
6.159	25	120	14.37
5.142	25	211	17.23
4.911	5	002	18.05
4.629	3	012	19.16
4.375	16	112	20.28
4.182	4	031	21.23
4.066	10	301	21.84
3.962	100	202	22.42
3.906	25	311	22.75
3.839	18	122	23.15
3.807	18	212	23.35
3.756	40	320	23.67
3.548	8	231	25.08
3.464	85	040	25.70
3.352	8	140,400	26.57
3.264	9	041,132	27.30
3.179	7	103,141	28.05
3.092	25	411	28.85
3.051	7	331	29.25
3.009	10	232	29.67
2.984	10	322	29.92
2.938	3	241	30.40
2.883	8	421	30.99
2.832	1	042	31.57
2.768	16	142,402	32.32
2.736	6	340	32.70
2.707	8	223	33.06
2.666	5	051	33.59
2.638	14	341	33.96
2.615	25	151,431	34.26
2.608	16	242	34.36
2.541	2	511	35.30
2.498	4	520	35.92
2.477	4	251	36.23
2.456	5	004	36.56
2.379	4	114,043 +	37.79
2.338	4	441	38.47
2.306	13	204	39.03
2.277	20	160,214	39.55
2.243	6	243	40.18
2.228	11	522	40.46
2.183	2	260	41.32
2.161	6	442	41.76
2.119	2	540	42.63
2.087	5	433,451	43.31
2.065	6	162	43.80
2.050	10	360,513	44.14
2.033	5	602	44.53
2.004	2	044	45.20
1.980	4	144,404	45.79
1.958	1	452	46.33
1.941	3	071,443	46.77
1.921	6	171,244	47.29
1.891	8	025,551 +	48.08
1.866	4	461	48.75
1.861	5	711,632	48.89
1.845	2	720,641	49.36
1.828	4	613,344	49.85
1.780	7	371,543	51.28
1.752	3	642,524	52.16
1.749	2	560	52.26
1.733	3	080	52.78
1.727	3	722	52.99
1.710	2	045	53.56

Lead chloride fluoride (matlockite), PbClF

Sample
The sample was prepared by melting a 1:1 molar mixture of $PbCl_2$ and PbF_2 at about 600 °C.

Color
Yellowish gray

Structure
Tetragonal, P4/nmm (129), Z = 2, isostructural with BaClF and other similar double halides. The structure of PbClF was determined by Bannister [1934].

NBS lattice constants of this sample:

a = 4.1104(2)Å
c = 7.2325(5)

Density
(calculated) 7.111 g/cm^3

Reference intensity
$I/I_{corundum}$ = 6.2

Additional patterns
1. PDF card 4-460 [Swanson et al., 1953].
2. Nieuwenkamp and Bijvoet [1932].

References
Bannister, F.A. (1934). Mineral. Mag. 23, 587.
Nieuwenkamp, W. and Bijvoet, J. M. (1932). Z. Krist. 81, 469.
Swanson, H. E. and Tatge, E. (1953). Nat. Bur. Stand. (U.S.) Circ. 539, 1, 76.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
7.22	13	001	12.25
3.617	40	002	24.59
3.574	100	101	24.89
2.906	45	110	30.74
2.715	35	102	32.96
2.412	4	003	37.25
2.265	40	112	39.76
2.079	16	103	43.49
2.055	20	200	44.04
1.976	2	201	45.88
1.855	9	113	49.06
1.808	1	004	50.43
1.786	17	202	51.10
1.781	25	211	51.26
1.6552	11	104	55.47
1.6386	9	212	56.08
1.5636	2	203	59.03
1.5350	1	114	60.24
1.4618	7	213	63.60
1.4528	5	220	64.04
1.4466	3	005	64.35
1.4249	1	221	65.45
1.3645	1	105	68.74
1.3478	5	222	69.71
1.3458	4	301	69.83
1.3001	5	310	72.67
1.2952	6	115	72.99
1.2891	8	214	73.39
1.2814	2	302	73.90
1.2232	5	312	78.06
1.1910	1	303	80.60
1.1831	3	205	81.25
1.1567	2	106	83.51
1.1440	2	313	84.65
1.1368	1	215	85.31
1.1259	2	321	86.34
1.0920	2	304	89.72
1.0873	2	322	90.22
1.0331	1	007	96.43
1.0252	2	225	97.42
1.0079	1	216	99.68
0.9878	2	411	102.49
.9736	1	117	104.59
.9669	2	315	105.63
.9645	3	324	106.01

Magnesium phosphate, $Mg(PO_3)_2$

Sample
The sample was prepared by heating a 1:2 molar mixture of $MgCO_3$ and H_3PO_4 to 710 °C. It was then reground and reheated at 710 °C several times.

Color
Colorless

Structure
Monoclinic, I2/a(15) or Ia(9), Z=8 [Beucher and Grenier, 1968]. Those authors gave the cell in the settings C2/c(15) or Cc(9).

NBS lattice constants of this sample:

a = 11.119(3)Å
b = 8.268(2)
c = 9.920(3)
β = 112.44(3)°

Density
(calculated) 2.872 g/cm^3

Reference intensity
$I/I_{corundum}$ = 1.4

Additional pattern
1. PDF card 11-41 [Sarver and Hummel, 1959].

References
Beucher, M. and Grenier, J.-C. (1968). Mater. Res. Bull. 3, 643.
Sarver, J. F. and Hummel, F. A. (1959). J. Electrochem. Soc. 106, 500.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
6.44	2	110	13.75
6.14	16	011	14.42
5.13	4	200	17.26
4.59	60	002	19.34
4.34	4	$\bar{2}02$	20.47
4.243	35	$\bar{1}12$	20.92
3.731	1	$\bar{1}21$	23.83
3.519	20	211	25.29
3.371	25	112,121	26.42
3.219	50	220	27.69
3.181	30	$\bar{3}12$	28.03
3.164	30	310	28.18
3.070	2	022	29.06
2.993	100	$\bar{2}22$	29.83
2.865	16	013	31.19
2.728	6	$\bar{4}02$	32.80
2.662	1	130	33.64
2.576	20	$\bar{1}23$	34.80
2.380	16	222	37.77
2.373	12	$\bar{3}23$	37.89
2.358	6	321	38.14
2.277	6	$\bar{4}22,\bar{3}14$	39.55
2.248	4	231	40.07
2.242	3	123	40.19
2.181	8	420,411	41.37
2.147	2	330	42.05
2.094	17	$\bar{2}33$	43.16
2.068	2	040	43.74
1.946	3	141,402	46.63
1.938	3	$\bar{5}21$	46.85
1.929	4	$\bar{2}15$	47.07
1.885	3	042	48.23
1.865	2	$\bar{2}42$	48.78
1.848	2	$\bar{4}33,204$	49.27
1.828	2	$\bar{1}34$	49.83
1.805	4	$\bar{3}41$	50.53
1.796	6	$\bar{3}34$	50.81
1.755	6	$\bar{1}25$	52.06
1.754	6	233	52.10
1.751	4	$\bar{1}43$	52.19
1.728	6	$\bar{5}32$	52.96
1.692	7	$\bar{6}22$	54.18
1.648	4	442,530	55.74
1.627	7	051	56.51
1.623	8	512	56.67
1.6102	10	440	57.16
1.5353	8	044	60.23
1.5184	6	$\bar{6}33$	60.97
1.5148	6	$\bar{6}31$	61.13
1.4974	4	$\bar{4}44$	61.92

Magnesium tungsten oxide, $MgWO_4$

Sample
The sample was prepared by treating an aqueous solution of Na_2WO_4 with concentrated $MgCl_2$ at 80°C. The precipitate was filtered, washed with alcohol and heated at 850°C for 30 minutes.

Color
Colorless

Structure
Monoclinic, P2/a (13), Z=2, isostructural with wolframite, $(Fe,Mn)WO_4$ [Broch, 1929].

NBS lattice constants of this sample:

a = 4.9288(6)Å
b = 5.6751(8)
c = 4.6879(5)
β = 90.70(1)°

Density
(calculated) 6.893 g/cm^3

Reference intensity
$I/I_{corundum}$ = 3.0

Polymorphism
The monoclinic, wolframite type reported here is stable below 1165°C. Chang et al.[1966] reported a high temperature modification stable above 1165°C. Their data are given on PDF card 19-776. Dunning et al., [1947] reported the existence of a cubic modification, formed between 90° and 300°C.

Additional patterns
1. PDF card 7-190 [Swanson et al. 1953].
2. Broch [1929].
3. Dunning and Megaw [1946].
4. Fonda [1944].

References

Broch, E.(1929). Skrifter Norske Videns. - Akad., Oslo I. Mat. Nat. Klasse 1929, No. 8.
Chang, L. L. Y., Scroger, M. G., and Phillips, B. (1966). J. Amer. Ceram. Soc. 49, 385.
Dunning, N. J. and Megaw, H. D., (1946). Trans. Faraday Soc. 42, 705.
Fonda, G. R. (1944). J. Phys. Chem. 48, 303.
Swanson, H. E. and Tatge, E. (1953). Nat. Bur. Stand., U.S. Circ. 539, Vol. I, 84.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
5.67	20	010	15.63
4.68	95	001	18.94
3.719	100	110	23.91
3.610	45	011	24.64
2.929	100	$\bar{1}11$	30.50
2.901	95	111	30.80
2.836	25	020	31.52
2.463	40	200	36.45
2.459	40	120	36.51
2.427	18	021	37.01
2.343	20	002	38.39
2.261	3	$\bar{2}10$	39.84
2.191	25	$\bar{2}01$	41.16
2.185	14	$\bar{1}21$	41.28
2.172	40	121,201	41.55
2.044	6	$\bar{2}11$	44.28
2.027	11	211	44.68
1.9919	13	$\bar{1}12$	45.50
1.9751	18	112	45.91
1.8913	8	030	48.07
1.8600	13	220	48.93
1.8068	12	022	50.47
1.7660	3	130	51.72
1.7540	25	031	52.10
1.7346	6	$\bar{2}21$	52.73
1.7243	7	221	53.07
1.7087	15	$\bar{2}02$	53.59
1.7020	17	$\bar{1}22$	53.82
1.6909	20	122	54.20
1.6881	25	202	54.30
1.6552	2	$\bar{1}31$	55.47
1.6508	2	131	55.63
1.6360	2	$\bar{2}12$	56.18
1.6180	2	212	56.86
1.5782	7	310	58.43
1.5626	4	003	59.07
1.5061	3	$\bar{0}13$	61.52
1.5011	18	$\bar{3}11$,230	61.75
1.4904	10	311	62.24
1.4720	7	032	63.11
1.4643	6	$\bar{2}22$	63.48
1.4508	6	222	64.14
1.4458	11	$\bar{1}13$	64.39
1.4360	14	113	64.88
1.4327	17	$\bar{2}31$	65.05
1.4264	12	231	65.37
1.4222	15	320	65.59
1.3690	3	$\bar{0}23$	68.48
1.3641	13	$\bar{3}21$,140	68.76
1.3565	4	321	69.20

Magnesium tungsten oxide, $MgWO_4$

d(Å)	I	hkℓ	2θ(°)
1.3271	2	$\bar{2}03$	70.96
1.3224	6	$\bar{1}23$	71.25
1.3160	4	$\bar{3}12$	71.65
1.3121	7	$20\bar{3}$	71.90
1.3102	8	$\bar{1}41$	72.02
1.3019	4	$3\bar{1}2$	72.55
1.2923	2	$\bar{2}13$	73.17
1.2786	2	$2\bar{1}3$	74.09
1.2681	4	$\bar{2}32$	74.81

Mercury chloride, $HgCl_2$

Sample
The sample was commercially prepared mercuric chloride.

Color
Colorless

Optical data
Biaxial(-), $N_\alpha = 1.725$, $N_\beta = 1.859$, $N_\gamma = 1.965$, $2V = 85°$ [Merwin, 1920].

Structure
Orthorhombic, Pmnb (62), Z = 4. The structure was determined by Braekken and Scholten [1934].

NBS lattice constants of this sample:

a = 5.9756(8) Å
b = 12.768(2)
c = 4.3347(6)

Density
(calculated) 5.453 g/cm^3

Reference intensity
$I/I_{corundum} = 3.2$

Additional pattern
1. PDF card 4-331 [Swanson and Tatge, 1953].

References

Braekken, H. and Scholten, W. (1934). Z. Krist. 89, 448.
Merwin, H.E. (1920). J. Am. Chem. Soc. 42, 2432.
Swanson, H. E. and Tatge, E. (1953). Nat. Bur. Stand. (U.S.) Circ. 539, 1, 73.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
4.365	100	120	20.33
4.107	40	011	21.62
3.587	7	021	24.80
3.511	5	101	25.35
3.386	10	111	26.30
3.192	12	040	27.93
3.075	12	121	29.01
3.038	30	031	29.38
2.989	50	200	29.87
2.708	40	131,220	33.05
2.418	20	211	37.16
2.361	4	141	38.08
2.295	3	221	39.22
2.199	8	051	41.01
2.181	6	240	41.36
2.130	14	231,060	42.41
2.065	16	151	43.81
2.012	10	112	45.01
2.006	16	160	45.16
1.941	13	122	46.76
1.902	7	320	47.78
1.838	2	132	49.55
1.820	1	161	50.09
1.810	1	301	50.38
1.793	10	042,311	50.90
1.771	4	251	51.56
1.754	3	202	52.09
1.740	2	321	52.54
1.738	2	212	52.61
1.681	3	071	54.55
1.666	5	331	55.09
1.653	2	052	55.55
1.621	4	232	56.73
1.618	3	171	56.85
1.595	4	080	57.74
1.574	1	341	58.61
1.537	5	242	60.15
1.493	3	400	62.10
1.477	3	351	62.87
1.472	4	162	63.09
1.454	4	420,360	63.98
1.436	1	013	64.89
1.429	4	322	65.22
1.408	3	280	66.32
1.4043	5	103,411	66.53
1.3958	2	113,072	66.99
1.3788	<1	421,361	67.93
1.3538	1	262	69.36
1.3406	2	431	70.14
1.3151	1	191	71.71
1.2939	1	213	73.07
1.2850	2	082,371	73.66
1.2745	1	223	74.37
1.2360	1	451	77.10
1.2304	2	153,402	77.52
1.1805	1	282	81.46
1.1748	1	520	81.94
1.1694	1	303	82.40
1.1648	1	313	82.80
1.1478	2	442,511	84.31

Mercury chloride (calomel), Hg_2Cl_2

Sample
The sample was obtained from British Drug House, Ltd.

Optical data
Uniaxial(+), N_o = 2.6559, N_e = 1.97325 [Groth, 1904].

Structure
Tetragonal, I4/mmm (139), Z = 2, isostructural with Hg_2Br_2, Hg_2F_2, and Hg_2I_2 [Havighurst, 1925 and Mark and Steinback, 1926].

NBS lattice constants of this sample:

a = 4.4801(2)Å
c = 10.9060(6)

Density
(calculated) 7.162 g/cm^3

Reference intensity
$I/I_{corundum}$ = 5.0

Additional patterns
1. PDF card 4-581 [Swanson and Tatge, 1953].
2. Havighurst [1925].
3. Hylleraas [1926].
4. Ruff et al. [1928].
5. Hanawalt et al. [1938].

References

Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Havighurst, R.J. (1925). Amer. J. Sci. 10, 15.
Hylleraas, E. (1926). Z. Phys. 36, 859.
Groth, H. (1904). Chemische Krystallographie, Vol. 1, 124, Engelmann, Leipzig.
Mark, H. and Steinbach, J. (1926). Z. Krist. 64, 79.
Ruff, O., Ebert, F., and Luft, F. (1928). Z. Anorg. Allg. Chem. 170, 49.
Swanson, H.E. and Tatge, E. (1953). NBS Circular 539, 1, 72.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
4.147	75	101	21.41
3.170	100	110	28.13
2.824	12	103	31.66
2.727	30	004	32.81
2.240	15	200	40.22
2.067	40	114	43.76
1.970	17	211	46.03
1.962	30	105	46.24
1.818	<1	006	50.14
1.756	4	213	52.05
1.732	12	204	52.83
1.5841	6	220	58.19
1.4755	11	215	62.94
1.4164	3	310	65.89
1.3815	1	303	67.78
1.3696	6	224	68.45
1.3633	3	008	68.81
1.2569	4	314	75.59
1.2522	5	118	75.93
1.2343	2	321	77.23
1.2319	2	305	77.41
1.1756	1	323	81.88
1.1697	5	109	82.38
1.1648	3	208	82.80
1.1202	<1	400	86.89
1.0908	<1	0·0·10	89.85
1.0800	2	325	91.00
1.0563	1	330	93.65
1.0410	1	413	95.46
1.0370	3	219,332	95.95
1.0312	2	1·1·10	96.66
1.0018	1	420	100.52
0.9846	2	334	102.95
.9823	2	318	103.29
.9728	2	415	104.72
.9405	1	424	109.97
.9089	1	0·0·12	115.89
.8930	<1	431	119.22
.8736	1	1·1·12	123.72
.8675	2	329	125.23
.8287	1	435	136.71
.8246	2	1·0·13	138.20

Nickel acetate hydrate, $Ni(C_2H_3O_2)_2 \cdot 4H_2O$

Sample
The sample was prepared by slow evaporation at room temperature of an aqueous solution of $Ni(C_2H_3O_2)_2$.

Color
Brilliant bluish green.

Optical data
Biaxial (-). N_α = 1.441, N_γ = 1.560. 2V is very small.

Structure
Monoclinic $P2_1/c(14)$, Z = 2, isostructural with $Co(C_2H_3O_2)_2 \cdot 4H_2O$. The structure was determined by van Niekerk and Schoening [1953] and refined by Downie et al. [1971].

NBS lattice constants of this sample:

a = 4.7749(9) Å
b = 11.772(2)
c = 8.435(1)
β = 93.86(1)°

Density
(calculated) 1.747 g/cm^3

Reference intensity
$I/I_{corundum}$ = 4.6

Additional patterns
1. PDF card 14-721 [Hanawalt et al., 1938].
2. PDF card 24-1360. This is data from card 14-721 indexed by University College, Cardiff, Wales.

References
Downie, T. C., Harrison, W., Rafer, E. S., and Hepworth, M. A. (1971). Acta Crystallogr. B27, 706.
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
van Niekerk, J. N. and Schoening, F. R. (1953). Acta Crystallogr. 6, 609.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
6.84	100	011	12.94
5.886	4	020	15.04
4.828	6	021	18.36
4.762	30	100	18.62
4.416	2	110	20.09
4.209	13	002	21.09
4.014	19	$\bar{1}11$	22.13
3.962	5	012	22.42
3.811	7	111	23.32
3.702	<1	120	24.02
3.555	11	031	25.03
3.454	<1	$\bar{1}21$	25.77
3.326	2	121	26.78
3.265	2	$\bar{1}02$	27.29
3.147	20	$\bar{1}12$	28.34
3.053	3	102	29.23
3.029	2	130	29.47
2.956	4	112	30.21
2.946	2	040	30.32
2.890	8	$\bar{1}31$	30.92
2.869	7	032	31.15
2.813	1	131	31.79
2.711	5	122	33.02
2.531	1	023	35.44
2.504	8	140	35.83
2.438	2	$\bar{1}13$	36.83
2.410	3	042,132	37.28
2.383	2	200	37.72
2.378	4	141	37.80
2.304	7	113	39.07
2.294	7	$\bar{1}23$	39.24
2.281	2	033	39.47
2.267	1	051	39.70
2.186	5	$\bar{1}42$,123	41.27
2.136	1	$\bar{2}02$	42.27
2.111	5	150	42.81
2.104	4	004,$\bar{2}21$,$\bar{1}33$	42.95
2.063	3	$\bar{1}51$	43.85
2.055	2	052	44.04
2.032	1	151,043	44.56
2.016	3	$\bar{2}02$,133	44.92
2.007	4	$\bar{2}22$	45.13
1.982	1	024	45.75
1.953	1	231	46.46
1.948	2	$\bar{1}14$	46.59
1.907	3	222	47.64
1.879	2	$\bar{1}04$	48.41
1.875	2	$\bar{2}32$	48.51
1.872	2	$\bar{1}24$	48.61
1.855	6	$\bar{2}13$,114,034	49.06

Nickel acetate hydrate, $Ni(C_2H_3O_2)_2 \cdot 4H_2O$ - continued

d(Å)	I	hkℓ	2θ(°)
1.852	5	240	49.16
1.836	1	143	49.61
1.803	2	053	50.57
1.791	3	$\bar{2}23$	50.95
1.789	2	124,241	51.01
1.778	3	062	51.36
1.7645	<1	161,$\bar{1}$34	51.77
1.7392	2	213	52.58
1.7282	1	$\bar{2}42$	52.94
1.7108	<1	044,$\bar{1}$53	53.52
1.6944	2	$\bar{2}33$,134	54.08
1.6812	<1	$\bar{1}62$	54.54
1.6660	2	015	55.08
1.6629	2	242,153	55.19
1.6272	1	251	56.51
1.6074	2	063,$\bar{1}$15	57.27
1.6043	1	233	57.39

Potassium lead chloride, KPb_2Cl_5

Sample
The sample was prepared by melting a 1:2 molar mixture of KCl and $PbCl_2$ at 480 °C and cooling in air.

Color
Colorless

Structure
Orthorhombic, Z=4, isostructural with $RbPb_2Cl_5$ and other similar compounds [Jansen, 1968].

NBS lattice constants of this sample:

a = 8.865(2) Å
b = 12.498(2)
c = 7.934(1)

Density
(calculated) 4.767 g/cm^3

Additional pattern
1. PDF card 23-484 [Jansen, 1968].

Reference
Jansen, P. W. J. (1968). Rec. Trav. Chim. Pays-Bas, 87, 1021.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
8.83	25	100	10.01
6.69	11	011	13.22
6.25	5	020	14.16
5.90	7	101	15.00
5.34	11	111	16.58
5.10	10	120	17.37
4.292	7	121	20.68
3.968	25	002	22.39
3.693	100	211,031	24.08
3.616	40	102,220	24.60
3.478	8	112	25.59
3.406	9	131	26.14
3.350	2	022	26.59
3.290	3	221	27.08
3.129	5	122	28.50
3.478	8	112	25.59
3.406	9	131	26.14
3.350	2	022	26.59
3.290	3	221	27.08
3.129	5	122	28.50
3.123	3	040	28.56
2.952	4	202,300	30.25
2.907	4	041	30.73
2.876	11	310,032	31.07
2.836	6	231	31.52
2.764	9	141	32.36
2.733	9	132	32.74
2.703	<2	311	33.11
2.671	50	222,320	33.52
2.587	5	013	34.65
2.553	20	240	35.12
2.534	9	103	35.39
2.483	2	113	36.14
2.454	2	042	36.59
2.371	4	302	37.91
2.350	14	123	38.27
2.328	7	312	38.65
2.303	10	151	39.09
2.232	18	033	40.38
2.216	16	400,322	40.68
2.166	6	133	41.67
2.148	8	242,340	42.04
2.101	19	251	43.02
2.083	7	060	43.41
2.059	5	332	43.94
2.027	3	160	44.66
1.994	3	233	45.44
1.968	7	143	46.08
1.935	9	104,402	46.92
1.912	5	114,412	47.51
1.900	13	431	47.84
1.879	6	323	48.40
1.856	<2	351	49.04
1.848	5	422	49.27
1.845	9	062	49.36
1.817	<2	053	50.18
1.810	5	204	50.38
1.805	3	162	50.51
1.781	4	333	51.24
1.762	<2	441	51.84
1.756	3	510,134	52.04
1.740	3	224	52.56
1.680	2	253	54.58
1.6679	3	521	55.01
1.6467	2	304	55.78
1.6330	<2	314	56.29
1.6232	2	451	56.66
1.6190	2	502	56.82
1.6092	3	163	57.20
1.5730	5	433	58.64
1.5624	2	080,105	59.08
1.5314	3	334	60.40
1.5177	4	460	61.00
1.5155	5	125	61.10

Potassium platinum chloride, K_2PtCl_6

Sample
The sample was prepared by reaction of KCl and H_2PtCl_6.

Major impurities

0.01 to 0.1% Na and Ba
0.001 to 0.01% Al, Ca, Cr, and Si
0.0001 to 0.001% Ag, Fe, Mg, and Mn

Color
Bright yellow

Optical data
Isotropic, N = 1.823

Structure
Cubic, Fm3m (225) Z=4, isostructural with other similar alkali platinum halides. The structure of K_2PtCl_6 was determined by Ewing and Pauling [1928].

NBS lattice constant of this sample:

$a = 9.7560(1)$ Å

Density
(calculated) 3.478 g/cm^3

Reference intensity
$I/I_{corundum} = 5.7$

Additional patterns
1. PDF card 7-199 [Swanson et al., 1955].
2. Hanawalt et al. [1938].

References
Ewing, F.J. and Pauling, L. (1928). Z. Krist. 68, 223.
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Swanson, H. E., Gilfrich, N.T., and Ugrinic, G.M. (1955). Nat. Bur. Stand. (U.S.) Circ. 539, 5, 49.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
5.633	100	111	15.72
4.878	40	200	18.17
3.4491	45	220	25.81
2.9417	45	311	30.36
2.8160	5	222	31.75
2.4391	40	400	36.82
2.2383	13	331	40.26
2.1817	15	420	41.35
1.9915	14	422	45.51
1.8773	14	511	48.45
1.7246	18	440	53.06
1.6492	13	531	55.69
1.6259	6	600	56.56
1.5425	5	620	59.92
1.4878	4	533	62.36
1.4083	4	444	66.32
1.3659	6	711	68.66
1.3531	3	640	69.40
1.3035	4	642	72.45
1.2700	4	731	74.68
1.2194	1	800	78.35
1.1918	1	733	80.53
1.1829	2	820	81.26
1.1496	1	660	84.14
1.1264	2	751	86.29
1.0907	3	840	89.86
1.0708	2	911	92.00
1.0645	2	842	92.71
1.0401	1	664	95.57
1.0226	2	931	97.75
0.9957	2	844	101.36
.9805	2	933	103.56
.9757	1	10·0·0	104.28
.9567	2	10·2·0	107.25
.9431	2	951	109.49
.9098	1	953	115.71
.9059	2	10·4·0	116.50
.8905	1	10·4·2	119.76
.8796	1	11·1·1	122.26
.8624	1	880	126.57
.8525	1	11·3·1	129.28
.8492	1	10·4·4	130.22
.8366	1	10·6·0	134.08
.8275	1	11·3·3	137.14
.8130	1	12·0·0	142.69
.8064	1	11·5·1	146.40
.7912	1	12·2·2	153.60
.7835	<1	11·5·3	158.90

Silicon, Si

Sample
The sample was very pure vacuum floated, zone refined silicon. This sample is NBS Standard Reference Material # 640, Silicon Powder, X-Ray Diffraction Standard.*

Major impurities (after grinding of the sample):

0.001-0.0001% each of Ca, Cu.

Color
Gray

Structure
Cubic, Fd3m (227), Z = 8 [Debye and Scherrer, 1916].

NBS lattice constant of this sample:

$a = 5.43088(4)\,\text{Å}$

Density
(calculated) 2.329 g/cm^3

Reference intensity
$I/I_{corundum} = 4.7$

Polymorphism
Kasper and Richards [1964] reported that a second, dense form with space group Ia3(206) is formed under pressure.

Additional pattern
1. PDF card 5-565 [Swanson and Fuyat, 1953]. The Swanson and Fuyat [1953] reference lists a large number of early powder patterns.

References

Debye, P. and Scherrer, P. (1916). Phys. Z. 17, 277.
Kasper, J. S. and Richards, S. M. (1964). Acta Crystallogr. 17, 752.
Swanson, H. E. and Fuyat, R. K. (1953). Nat. Bur. Stand. (U.S.) Circ. 539, 2, 6.

*Samples may be obtained from the Office of Standard Reference Materials, Room B311, Chemistry Building, National Bureau of Standards, Washington, D. C. 20234, $52 per 10 gram unit.

$CuK\alpha_1$ $\lambda = 1.540598$ Å; temp. 25±1 °C

Internal standard W, $a = 3.16524$ Å

d(Å)	I	hkℓ	2θ(°)
3.13552	100	111	28.443
1.92011	55	220	47.303
1.63747	30	311	56.123
1.35772	6	400	69.131
1.24593	11	331	76.377
1.10857	12	422	88.032
1.04517	6	511	94.954
0.96005	3	440	106.710
.91799	7	531	114.094
.85870	8	620	127.547
.82820	3	533	136.897

Silver carbonate, Ag_2CO_3

Sample
The sample was prepared by precipitation, adding K_2CO_3 to $AgNO_3$ solution.

Major impurities

0.001 to 0.01%, Al and Si
0.0001 to 0.001%, Ca, Cu, Fe, and Mg

Color
Greenish yellow

Structure
Monoclinic, $P2_1(4)$, Z=2 [Donahue and Helmholz, 1944].

NBS lattice constants of this sample:

a = 4.8510(7) Å
b = 9.544(2)
c = 3.2533(6)
β = 91.96°(2)

Density
(calculated) 6.084 g/cm^3

Additional patterns
1. PDF card 12-766 [Swanson et al., 1962].
2. Hanawalt et al [1938].

References

Donahue, J. and Helmholz, L. (1944). J. Am. Chem. Soc. 66, 295.

Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.

Swanson, H. E., Morris, M.C., Stinchfield, R. P., and Evans, E.H. (1962). Nat. Bur. Stand. (U.S.) Monogr. 25, Sec. 1, 44.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
4.85	15	100	18.29
4.78	35	020	18.56
4.32	30	110	20.52
3.41	2	120	26.14
3.252	3	001	27.40
3.078	8	011	28.99
2.745	60	$\bar{1}01$	32.60
2.660	100	130,101	33.66
2.561	6	111	35.01
2.423	2	200	37.07
2.385	11	040	37.68
2.381	13	$\bar{1}21$	37.76
2.351	8	210	38.26
2.322	14	121	38.75
2.275	35	031	39.59
2.161	11	220	41.76
2.041	10	$\bar{1}31$	44.35
1.976	2	$\bar{2}01$	45.89
1.935	6	$\bar{2}11$	46.92
1.929	9	230	47.08
1.912	4	201	47.51
1.875	6	$\bar{2}11$	48.52
1.801	3	$\bar{1}41$	50.65
1.777	13	150,141	51.39
1.701	3	240	53.87
1.678	9	$\bar{2}31$	54.65
1.646	6	051	55.82
1.639	10	231	56.07
1.626	6	002	56.56
1.616	1	300	56.92
1.591	9	060	57.93
1.538	2	022,$\bar{1}$12	60.11
1.530	3	320	60.44
1.526	3	102	60.64
1.511	2	160	61.29
1.507	3	$\bar{1}12$	61.47
1.4676	<1	$\bar{3}01$	63.32
1.4526	<1	$\bar{1}22$	64.05
1.4500	1	$\bar{3}11$	64.18
1.4412	2	330	64.62
1.4278	1	301	65.30
1.4115	1	$\bar{3}11$	66.15
1.3987	5	$\bar{1}32$	66.83

Silver sulfate, Ag_2SO_4

Sample
The sample was obtained from J. T. Baker Chemical Company.

Major impurities

0.001 to 0.01% each of Al, Fe, Mg, and Si.
0.0001 to 0.001% each of Ca and Pb.

Color
Colorless

Optical data
Biaxial (-), N_α=1.756, N_β=1.775, and N_γ= 1.782.

Structure
Orthorhombic, Fddd(70), Z=8, Na_2SO_4 type structure [Herrmann and Ilge, 1931].

NBS lattice constants of this sample:

a = 10.2699(5)Å
b = 12.7069(7)
c = 5.8181(3)

Density
(calculated) 5.455 g/cm^3

Reference intensity
$I/I_{corundum}$ = 2.2

Additional patterns
1. PDF card 7-203 [Swanson et al., 1957].
2. Hanawalt et al. [1938].

References

Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem., Anal. Ed. 10, 457.

Herrmann, K. and Ilge, W. (1931). Z. Krist. 80, 402.

Swanson, H. E., Gilfrich, N. T., and Cook, M. I. (1957). Nat. Bur. Stand. (U.S.) Circ. 539, 7, 46.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
4.699	10	111	18.87
3.994	25	220	22.24
3.249	3	131	27.43
3.177	70	040	28.06
2.873	100	311	31.10
2.644	90	022	33.87
2.568	1	400	34.91
2.530	17	202	35.45
2.421	30	331	37.10
2.352	3	222	38.24
2.272	8	151	39.64
1.980	11	242	45.78
1.957	8	260	46.35
1.926	30	351	47.15
1.915	12	511	47.44
1.884	5	113	48.26
1.762	3	531	51.85
1.7376	3	133	52.63
1.7123	17	062	53.47
1.6730	12	313	54.83
1.6527	4	620	55.56
1.6243	1	262	56.62
1.5881	3	080	58.03
1.5675	13	333	58.87
1.5462	8	371	59.76
1.5404	6	551	60.01
1.4751	4	602	62.96
1.4542	3	004	63.97
1.4057	6	353	66.46
1.3668	3	224	68.61
1.3598	1	191	69.01
1.3457	2	282	69.84
1.3380	6	642,533	70.30
1.3312	6	660	70.71
1.3225	6	044	71.25
1.2837	1	800	73.75
1.2736	3	391	74.43
1.2359	3	373	77.11
1.2331	3	2·10·0,553	77.32
1.1905	1	840	80.64
1.1678	1	264	82.54
1.1645	3	0·10·2	82.83
1.1549	1	822	83.67
1.1408	1	591	84.94
1.1154	1	911,135	87.36
1.1136	1	573	87.53
1.0975	2	315	89.15
1.0919	3	624	89.73
1.0829	4	393,931	90.69
1.0809	3	682	90.90

Silver sulfate, Ag_2SO_4 - continued

d(Å)	I	hkℓ	2θ(°)
1.0758	3	3·11·1	91.46
1.0727	3	084	91.80
1.0663	2	335	92.51
1.0589	1	0·12·0	93.34
1.0272	1	862	97.17
1.0246	1	951	97.49
1.0203	1	6·10·0	98.05
1.0138	1	10·2·0	98.89
1.0109	1	355	99.28
0.9976	1	593	101.10
.9920	1	5·11·1	101.88
.9820	2	664	103.33
.9586	1	026	106.95
.9531	1	3·11·3,971	107.84
.9419	1	375	109.74
.9407	1	2·10·4,555	109.94
.9279	1	3·13·1,4·12·2	112.23
.9210	1	844	113.51

Sodium phosphate hydrate, α-$Na_4P_4O_{12}\cdot 4H_2O$

Sample
The sample was prepared by H.M. Ondik by hydrolytic cleavage of the α form of P_2O_5 below 15 °C. The material was neutralized by NaOH, then purified by salting out with NaCl, followed by repeated recrystallizations with H_2O and ethanol.

Major impurities

0.001 to 0.01% each of Ba, Ca, Si, and Sr.

Color
Colorless

Optical data
Biaxial(+), N_α = 1.440, N_β = 1.458, N_γ = 1.476.

Structure
Monoclinic, $P2_1/a$ (14), Z=2. The structure of α-$Na_4P_4O_{12}\cdot 4H_2O$ was determined by Ondik et al. [1961].

NBS lattice constants of this sample:

a = 9.691(2)Å
b = 12.342(2)
c = 6.187(2)
β = 92.58(1)°

Density
(calculated) 2.156 g/cm^3

Polymorphism
Thilo and Ratz [1949] reported a β, high temperature form of $Na_4P_4O_{12}\cdot 4H_2O$.

Additional patterns
1. PDF card 11-15 [Swanson et al., 1960].
2. Bell et al. [1952].
3. Thilo and Ratz [1949].

References
Bell, R.N., Audrieth, L.F., and Hill, O.F.(1952). Ind. Eng. Chem. 44, 568.
Ondik, H. M., MacGillavry, C .H., and Block, S. (1961). Acta Crystallogr. 14, 555.
Swanson, H. E., Cook, M. I., Evans, E. H., and de Groot, J.H. (1960). Nat. Bur. Stand. (U.S.) Circ. 539, 10, 52.
Thilo, E. and Ratz, R. (1949). Z. Anorg. Allg. Chem. 260, 255.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
7.64	75	110	11.58
6.17	90	001,020	14.34
5.21	5	120	17.00
4.844	65	200	18.30
4.719	60	111	18.79
4.510	3	210	19.67
4.369	17	021	20.31
3.933	20	$1\bar{2}1$	22.59
3.894	2	$\bar{2}01$	22.82
3.805	95	220	23.36
3.728	25	201	23.85
3.572	8	211	24.91
3.424	10	031	26.00
3.295	100	$\bar{2}21$	27.04
3.255	70	$\bar{1}31$	27.38
3.194	20	221	27.91
3.133	19	230	28.47
3.122	19	310	28.57
3.089	25	002,040	28.88
2.938	9	140	30.40
2.827	70	$\bar{2}31$,112	31.62
2.760	19	022,041 +	32.41
2.739	20	311	32.67
2.685	18	$\bar{1}22$	33.34
2.669	7	$\bar{1}41$	33.55
2.638	14	141	33.95
2.633	15	321	34.02
2.602	7	240,$\bar{2}12$	34.44
2.554	14	202	35.11
2.539	35	330	35.32
2.418	18	$\bar{2}41$,$\bar{1}32$	37.16
2.392	8	150	37.57
2.375	8	410,132	37.85
2.360	5	222	38.10
2.293	5	051	39.26
2.253	40	420	39.98
2.247	25	$\bar{3}12$	40.10
2.222	16	151	40.56
2.199	11	250	41.01
2.185	16	411,042	41.29
2.170	5	232	41.59
2.148	5	312	42.02
2.146	3	$\bar{4}21$,$\bar{1}42$	42.08
2.120	4	$\bar{3}41$	42.62
2.115	5	142	42.71
2.087	4	430,$\bar{2}51$	43.32
2.060	2	003,251	43.92
2.015	8	$\bar{2}42$	44.94
2.001	6	$\bar{4}31$	45.29
1.996	1	$\bar{3}32$	45.40

Sodium phosphate hydrate, α-$Na_4P_4O_{12}\cdot 4H_2O$ - continued

d(Å)	I	hkℓ	2θ(°)
1.968	8	242	46.08
1.961	10	350	46.25
1.955	8	023,431	46.40
1.949	8	$\bar{4}02$	46.56
1.928	10	332,052 +	47.09
1.924	7	$\bar{4}12$	47.19
1.913	6	510	47.49
1.907	10	$\bar{1}61$	47.65
1.903	14	$\bar{2}13,\bar{1}52$ +	47.75
1.895	9	260	47.97
1.854	18	$\bar{3}51$	49.11
1.850	18	$\bar{5}11$	49.20
1.842	9	033	49.44
1.837	9	$\bar{4}41,\bar{3}42$	49.58
1.823	10	$\bar{1}33$	50.00
1.786	8	223,422	51.11
1.776	8	$\bar{2}52$	51.42
1.7547	6	$\bar{3}13$	52.08
1.7500	5	$\bar{5}21$	52.23
1.7456	6	$\bar{2}33$	52.37
1.7349	5	360,170	52.72
1.7123	3	043,062	53.47
1.6991	6	$\bar{2}33$,432 +	53.92
1.6806	12	$\bar{3}61$	54.56
1.6761	16	143,$\bar{3}52$	54.72

Strontium hydroxide, $Sr(OH)_2$

Sample
The sample was prepared by heating $Sr(OH)_2 \cdot 8H_2O$ for 24 hours at about 200 °C.

Color
Colorless

Structure
Orthorhombic, Pbnm (62), Z=4, [Bärnighausen and Weidlein, 1965]. The structure was determined by Grueninger and Bärnighausen [1969].

NBS lattice constants of this sample:

a = 6.1201(6) Å
b = 9.892(1)
c = 3.9193(5)

Density
(calculated) 3.405 g/cm^3

Reference intensity
$I/I_{corundum}$ = 2.7

Additional patterns
1. PDF card 18-1273 [Bärnighausen and Weidlein, 1965].
2. PDF card 19-1276 [Mercer and Miller, 1966]. This pattern is labeled as anhydrous but is for $Sr(OH)_2 \cdot H_2O$.
3. Berggren and Brown [1971].

References

Bärnighausen, H. and Weidlein, J. (1965). Acta Crystallogr. 19, 1048.

Berggren, G. and Brown, A. (1971). Acta Chem. Scand. 25, 1377.

Grueninger, H. W. and Bärnighausen, H (1969). Z. Anorg. Allgem. Chem. 368, 53.

Mercer, R. A. and Miller, R.P. (1966). J. Inorg. Nucl. Chem. 28, 61.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
5.19	55	110	17.06
4.94	25	020	17.94
3.846	40	120	23.11
3.300	40	101	27.00
3.130	100	111	28.49
3.068	25	021,200	29.08
2.922	25	210	30.57
2.903	45	130	30.78
2.745	5	121	32.59
2.602	2	220	34.44
2.473	25	040	36.30
2.343	45	211	38.38
2.293	10	140	39.26
2.244	2	230	40.16
2.168	10	221	41.62
2.091	25	041	43.23
1.998	3	310	45.36
1.979	6	141	45.81
1.959	20	002	46.31
1.947	50	231	46.62
1.886	17	320	48.21
1.834	6	112	49.68
1.822	3	022	50.03
1.810	15	301	50.38
1.780	1	311	51.29
1.746	6	122	52.35
1.735	1	330	52.73
1.727	2	241	52.97
1.6970	17	151	53.99
1.6615	6	250	55.24
1.6486	6	060	55.71
1.6280	11	212	56.48
1.6245	16	132	56.61
1.5735	5	340	58.62
1.5360	7	042	60.20
1.5304	6	400,251	60.44
1.5126	3	410	61.23
1.4898	4	142	62.27
1.4751	3	232,161	62.96
1.4608	5	341	63.65
1.4518	1	260	64.09
1.4109	1	411	66.18
1.3874	1	430	67.45
1.3768	2	170	68.04
1.3696	2	421	68.45
1.3589	8	322	69.06
1.3353	1	351	70.46
1.3080	3	431	72.16
1.3012	4	440	72.60
1.2992	4	171,332	72.73
1.2829	4	270	73.80
1.2672	8	252,113	74.87
1.2618	5	062	75.25

Strontium hydroxide hydrate $Sr(OH)_2 \cdot H_2O$

Sample

The sample was prepared by heating $Sr(OH)_2$ in a partly closed tube with about 1 ml H_2O at 100°C for 24 hours. The sample contained a small amount of $SrCO_3$. Because of this and the tendency to lose H_2O when exposed to air, the intensities may be slightly in error.

Color

Colorless

Structure

Orthorhombic, $Pb2_1m$ (26), Z = 2. Isostructural with $Eu(OH)_2 \cdot H_2O$ and $Ba(OH)_2 \cdot H_2O$ [Bärnighausen, 1966]. The structure of $Sr(OH)_2 \cdot H_2O$ was determined by Bärnighausen and Weidlein [1967].

NBS lattice constants of this sample:

a = 6.201(1)Å
b = 6.716(1)
c = 3.6483(6)

Density

(calculated) 3.053 g/cm^3

Reference intensity

$I/I_{corundum}$ = 0.8

Additional patterns

1. PDF card 19-1276 [Mercer and Miller, 1966]. This pattern was labeled as $Sr(OH)_2$
2. Bärnighausen [1966].
3. Berggren and Brown [1971].
4. Carlson [1954].
5. Lutz [1965].

References

Bärnighausen, H. (1966). Z. Anorg. Allgem. Chem. 342, 233.

Bärnighausen, H., and Weidlein, J. (1967). Acta. Crystallogr. 22, 252.

Berggren, G., and Brown, A. (1971). Acta. Chem. Scand. 25, 1377.

Carlson, E. T. (1954). J. Res. Nat. Bur. Stand. 53, 371.

Lutz, H. D. (1965). Z. Naturforsch. 20b, 61.

Mercer, R. A., and Miller, R. P.,(1966). J. Inorg. Nucl. Chem 28, 61.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
6.20	65	100	14.28
4.556	80	110	19.47
3.651	40	001	24.36
3.360	55	020	26.51
3.147	45	101	28.34
2.954	15	120	30.23
2.848	60	111	31.39
2.814	100	210	31.77
2.472	50	021	36.31
2.363	10	201	38.05
2.296	70	121	39.21
2.230	85	211	40.42
2.106	25	130	42.91
2.067	10	300	43.77
1.977	18	310	45.87
1.825	35	002,131	49.94
1.816	25	230	50.21
1.798	7	301	50.72
1.760	11	320	51.90
1.750	7	102	52.24
1.738	12	311	52.63
1.6938	11	112	54.10
1.6792	7	040	54.61
1.6248	25	231	56.60
1.6033	9	022	57.43
1.5854	8	321	58.14
1.5515	5	122	59.53
1.5500	7	400	59.60
1.5311	13	212	60.41
1.5186	6	330	60.96
1.4808	9	141	62.69
1.4266	7	401	65.36
1.4073	7	420	66.37
1.4024	8	331	66.62
1.3784	7	132	67.95
1.3678	3	302	68.55
1.3398	7	312	70.19
1.3124	11	150	71.88
1.3029	5	340	72.49
1.2862	8	232	73.58
1.2664	6	322	74.93
1.2396	4	500	76.83
1.2350	9	042,151	77.18

Strontium hydroxide hydrate, $Sr(OH)_2 \cdot 8H_2O$

Sample
The sample was prepared by treating $SrCO_3$ with HCl followed by NaOH at boiling temperatures. On cooling, the first crystals formed were removed, redissolved and reprecipitated by slow evaporation at room temperature.

Color
Colorless

Optical Data
Uniaxial (-), N_o = 1.497, N_e = 1.475

Structure
Tetragonal, P4/ncc (130), Z = 4. The structure was determined by Smith [1953].

NBS lattice constants of this sample:

a = 9.019(2)Å
c = 11.614(2)

Density
(calculated) 1.868 g/cm^3

Reference intensity
$I/I_{corundum}$ = 1.3

Additional patterns
1. PDF card 1-1263 [Hanawalt et al, 1938].
2. PDF card 2-1262 [Natta, 1928].
3. Berggren and Brown [1971].

References
Berggren, G., and Brown, A. (1971). Acta. Chem. Scand. 25, 1377.
Hanawalt, J.D., Rinn, R.W., and Frevel, L.K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Natta, G. (1928). Gazz. Chim. Ital. 58, 870.
Smith, H. G. (1953). Acta. Crystallogr. 6, 604.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
6.37	50	110	13.89
5.81	45	002	15.25
4.50	45	200	19.70
4.292	100	112	20.68
3.559	80	202	25.00
3.190	19	220	27.95
2.904	14	004	30.76
2.795	45	222,213	31.99
2.768	60	311	32.32
2.640	40	114	33.93
2.560	55	312	35.02
2.442	40	204	36.78
2.357	6	214	38.15
2.296	25	322,313	39.21
2.253	20	400	39.99
2.147	30	224	42.06
2.102	18	402,323	42.99
2.035	65	314	44.48
2.017	55	420	44.91
1.997	15	332	45.36
1.935	6	006	46.92
1.905	20	422,413	47.70
1.852	12	116	49.15
1.801	11	315	50.63
1.780	7	404	51.28
1.779	15	206	51.33
1.715	9	334	53.37
1.692	15	512	54.15
1.655	8	424,226	55.46
1.6020	13	316	57.48
1.5106	9	514	61.32
1.4950	8	532	62.03
1.4690	6	406	63.25
1.4518	10	008	64.09
1.4331	8	108	65.03
1.4263	12	620	65.37
1.4157	7	118	65.93
1.3964	10	426	66.96
1.3818	8	208	67.76
1.3648	7	534	68.72

Strontium silicate, Sr_3SiO_5

Sample

The sample was prepared by repeated grindings and heatings of a 3:1 molar mixture of $SrCO_3$ and silica gel. The temperature was about 1350 °C.

Color

Colorless

Structure

Tetragonal, P4/ncc (130), Z=4 [Mansmann, 1965]. The structure of Sr_3SiO_5 was studied by Dent Glasser and Glasser [1965].

NBS lattice constants for this sample:

a = 6.9476(3)Å
c = 10.7534(6)

Density

(calculated) 4.747 g/cm^3

Reference intensity

$I/I_{corundum}$ = 3.6

Additional patterns

1. PDF card 18-1282[Dear, Bull. Mat. Eng. Exp. Sta., 1957].
2. Eysel [1970].
3. Nurse [1952].

References

Dent Glasser, L.S. and Glasser, R.P. (1965). Acta Crystallogr. 18, 453.

Eysel, W. (1970). Neues Jahrb. Mineral. Montash. 1970, 534.

Mansmann,M. (1965). Z. Anorg. Allg. Chem. 339,52.

Nurse, R. W. (1952). J. Appl. Chem. (London) 2, 244.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
5.38	4	002	16.46
4.92	1	110	18.02
4.249	1	102	20.89
3.629	10	112	24.51
2.984	30	211	29.92
2.919	100	202	30.60
2.690	30	212,004	33.29
2.508	2	104	35.78
2.458	30	220	36.53
2.348	55	213	38.30
2.198	25	310	41.04
2.035	1	312,214	44.49
1.897	4	321	47.92
1.814	20	322,224	50.27
1.793	2	006	50.89
1.7683	9	215	51.65
1.7550	1	304	52.07
1.7370	1	400	52.65
1.7014	9	314	53.84
1.6840	3	116	54.44
1.6646	17	411	55.13
1.6530	3	402	55.55
1.6376	2	330	56.12
1.5926	16	206	57.85
1.5662	10	332,324	58.92
1.5535	4	420	59.45
1.5366	1	421,315	60.17
1.5250	12	413	60.68
1.4926	4	422	62.14
1.4589	4	404	63.74
1.4352	2	325	64.92
1.3982	1	334	66.86
1.3889	1	316	67.37
1.3772	4	217	68.02
1.3446	7	424,008	69.90
1.3262	7	415	71.02
1.3208	5	512	71.35
1.2961	1	118,433	72.93
1.2810	1	521	73.93
1.2571	2	406	76.29
1.2338	1	218	77.27
1.2279	1	440,416	77.71
1.2140	3	523	78.77
1.2090	3	336	79.16
1.2012	1	327	79.77
1.1974	2	442	80.08
1.1913	3	530	80.57
1.1790	4	228	81.59
1.1739	2	426	82.02
1.1674	2	435	82.58

Strontium silicate, Sr_3SiO_5 - continued

d(Å)	I	hkℓ	2θ(°)
1.1632	3	532,524 +	82.94
1.1579	2	600	83.40
1.1468	1	318	84.40
1.1352	6	417	85.46
1.1154	3	219	87.36
1.0891	7	534	90.03
1.0846	4	516	90.51
1.0761	4	622	91.42
1.0632	5	604,408	92.85
1.0504	<1	1•1•10,623 +	94.33
1.0388	1	338	95.72
1.0305	1	437	96.75
1.0272	3	2•0•10	97.16
1.0161	2	428,2•1•10	98.59
1.0133	1	446	98.96
1.0088	2	615	99.56
0.9922	1	536	101.85
.9747	2	419	104.43
.9686	1	545	105.36
.9662	2	438,3•1•10 +	105.74
.9597	<1	641	106.77
.9506	1	721	108.26
.9484	2	642	108.63
.9364	2	626	110.69
.9324	2	2•1•11	111.40
.9305	1	643	111.75

Tin hydrogen phosphate, $SnHPO_4$

Sample
The sample was made by T. H. Jordan of the American Dental Association Health Foundation. Tin Fluoride, SnF_2, was treated with H_3PO_4 at a pH of 2, followed by slight heating.

Color
Colorless

Structure
Monoclinic, $P2_1/a(14)$, Z = 4. The structure was determined by Berndt and Lamberg [1971].

NBS lattice constants of this sample:

a = 5.8307(8)Å
b = 13.617 (1)
c = 4.6145(6)
β = 98.73 (1)°

Density
(calculated) 3.937 g/cm^3

Reference Intensity
$I/I_{corundum}$ = 2.0.

Reference
Berndt, A. F. and Lamberg, R. (1971). Acta Crystallogr. B27, 1092.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
6.80	100	020	13.01
5.311	2	110	16.68
4.562	12	001	19.44
4.401	11	120	20.16
4.327	1	011	20.51
3.792	12	021	23.44
3.731	16	$\bar{1}11$	23.83
3.566	6	130	24.95
3.404	35	040	26.16
3.367	4	$\bar{1}21$	26.45
3.241	8	111	27.50
2.997	30	$\bar{1}21$	29.79
2.946	40	$\bar{1}31$	30.31
2.882	1	200	31.01
2.820	14	210	31.71
2.729	4	041	32.79
2.689	7	131	33.29
2.654	1	$\bar{2}20$	33.75
2.623	1	$\bar{2}01$	34.16
2.574	4	$\bar{2}11$	34.82
2.559	1	$\bar{1}41$	35.04
2.448	1	$\bar{2}21$	36.68
2.384	3	141	37.71
2.338	1	051	38.47
2.279	6	002	39.51
2.269	11	$\bar{2}31$,060	39.69
2.251	10	211,012	40.02
2.228	3	$\bar{1}51$	40.45
2.210	4	$\bar{1}12$	40.79
2.163	<1	022	41.72
2.111	1	160,151	42.80
2.077	1	$\bar{2}41$	43.53
2.032	10	061	44.55
2.008	6	$\bar{1}32$	45.11
1.979	9	250	45.82
1.936	3	$\bar{2}02$,122	46.90
1.918	2	$\bar{2}12$	47.36
1.894	6	042	47.99
1.889	6	$\bar{2}51$	48.12
1.878	2	161	48.44
1.863	1	$\bar{2}22$	48.84
1.848	3	320	49.28
1.843	4	132,170	49.41
1.808	4	$\bar{3}21$	50.43
1.789	1	071	51.01
1.783	1	260	51.19
1.769	2	330	51.62
1.748	5	052	52.28
1.737	6	$\bar{1}71$	52.64
1.681	2	171	54.53

d(Å)	I	hkℓ	2θ(°)
1.669	1	202,311	54.96
1.657	2	$2\bar{1}2$	55.42
1.643	3	$\bar{3}41$	55.93
1.632	3	180,321	56.32
1.609	3	062	57.22
1.578	2	$\bar{2}52$	58.44
1.5585	1	$\bar{1}81$	59.24
1.5514	1	$\bar{3}22$	59.54
1.5166	4	181	61.05
1.5081	2	162,341	61.43
1.4989	1	242	61.85
1.4802	1	072	62.72
1.4730	2	$\bar{2}62$	63.06
1.4634	1	190	63.52
1.4486	2	$\bar{1}33$	64.25
1.4432	1	$\bar{3}42$	64.52
1.4384	2	$\bar{4}01,\bar{2}03$	64.76
1.4303	1	$351,\bar{4}11$ +	65.17
1.4231	2	252	65.54
1.4092	2	$420,\bar{1}91$	66.27
1.3943	1	$\bar{1}43$	67.07
1.3878	3	043,123	67.43
1.3781	1	191	67.97
1.3738	1	$430,\bar{2}72$	68.21
1.3670	1	370	68.59
1.3615	1	0·10·0	68.91

Zinc borate, $Zn_4B_6O_{13}$

Sample
The sample was a phosphor preparation obtained from the Radio Corporation of America [Leverenz, 1944].

Color
Colorless

Structure
Cubic, $I\bar{4}3m(217)$, Z=2. The structure was determined by Smith et al. [1961], who found the formula to be $Zn_4O(BO_2)_6$.

NBS lattice constant of this sample:

$a = 7.4734(2)$ Å

Density
(calculated) 4.252 g/cm^3

Additional pattern
1. PDF card 14-2 [Swanson and Tatge, 1953]. The formula at that time was mistakenly given as ZnB_2O_4.

References

Leverenz, H.W. (1944). Proc. I.R.E. 32, 256.
Smith, P., García-Blanco, S., and Rivoir, L. (1961). An. Reál Soc. Españ. Fis. Quim. Madrid, A57, 263.
Swanson, H. E. and Tatge, E. (1953). Nat. Bur. Stand. (U.S.) Circ. 539, 1, 83.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
5.29	6	110	16.74
3.74	4	200	23.77
3.05	100	211	29.28
2.364	25	310	38.03
2.158	2	222	41.82
1.997	20	321	45.37
1.869	14	400	48.68
1.761	40	330	51.88
1.672	2	420	54.86
1.594	4	332	57.79
1.526	25	422	60.63
1.466	6	510	63.39
1.364	8	521	68.76
1.321	4	440	71.34
1.282	4	530	73.86
1.246	2	600	76.37
1.213	2	611	78.84
1.1818	2	620	81.36
1.1532	4	541	83.82
1.1026	2	631	88.64
1.0789	2	444	91.12
1.0569	2	710	93.58
1.0366	2	640	96.00
1.0170	4	721	98.48
0.9992	2	642	100.88
.9813	2	730	103.44
.9491	2	732	108.51
.9199	4	811	113.74
.9063	2	820	116.42
.8933	2	653	119.16
.8808	2	822	121.99
.8688	4	831	124.92
.8574	2	662	127.91
.8463	2	752	131.08
.8253	2	910	137.95
.8154	2	842	141.73
.8059	2	921	145.83
.7967	2	664	150.44
.7878	2	930	155.83

Zinc titanium oxide, $ZnTiO_3$

Sample

The sample was prepared by heating an equimolar mixture of $Zn(NO_3)_2$ and TiO_2 (anatase) for about two weeks at 900° with several remixings and regrindings. Because of the lack of thermal stability above 943° [Dulin and Rase, 1960], it was impossible to obtain complete reaction and the sample contained small amounts of rutile (TiO_2) and Zn_2TiO_4; therefore there may be a slight error in some intensities. Intensities calculated from the structure were in good agreement with the experimental values.

Color

Colorless

Structure

Hexagonal, $R\bar{3}$ (148), Z=6. $ZnTiO_3$ is isostructural with $FeTiO_3$ (ilmenite) and other similar titanates [Bartram and Slepetys, 1961].

NBS lattice constants of this sample:

$a = 5.0787(3)$ Å
$c = 13.927(1)$

Density

(calculated) 5.165 g/cm^3

Reference intensity

$I/I_{corundum} = 2.5$

Additional patterns

1. Bartram and Slepetys [1961].
2. Kubo and Kato [1963].

References

Bartram, S.F. and Slepetys, R.A. (1961). J. Amer. Ceram. Soc. 44, 493.

Dulin, F.H. and Rase, D.E. (1960). J. Amer. Ceram. Soc. 43, 125.

Kubo, T. and Kato, M. (1963). Kogyo Kagaku Zasshi 66, 404.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
4.63	1	003	19.14
4.191	3	101	21.18
3.717	20	012	23.92
2.729	100	104	32.79
2.540	75	110	35.31
2.355	1	015	38.18
2.321	1	006	38.76
2.228	20	113	40.45
2.173	3	021	41.52
2.097	1	202	43.10
1.860	35	024	48.94
1.813	1	107	50.29
1.713	35	116	53.43
1.651	1	211	55.64
1.619	11	018	56.83
1.500	25	214	61.80
1.466	25	300	63.41
1.428	1	125	65.31
1.399	1	303	66.84
1.3650	4	208	68.71
1.3276	8	1·0·10	70.93
1.3218	4	119	71.29
1.2760	1	217	74.27
1.2696	6	220	74.71
1.2396	2	306	76.84
1.2166	1	0·1·11	78.57
1.2020	6	128,312	79.71
1.1766	3	0·2·10	81.79
1.1512	7	134	84.00
1.1139	5	226	87.50
1.0862	1	042	90.33
1.0674	5	2·1·10	92.38
1.0558	2	1·1·12	93.71
1.0485	3	404	94.56
1.0069	<1	1·2·11	99.82
0.9990	3	318	100.90
.9816	<1	229	103.39
.9702	4	0·1·14	105.12
.9692	7	324	105.27
.9599	5	410	106.74
.9296	2	048	111.92
.9175	3	1·3·10	114.19
.9064	2	2·0·14	116.39
.8868	5	416	120.59

Cerium cobalt, $CeCo_2$

Structure
Cubic, Fd3m(227), Z=8, C15 type, isostructural with Cu_2Mg [Fülling et al., 1942].

Lattice constant: [Wernick and Geller, 1960]

$a = 7.161(5)\text{Å}$

Density
(calculated) 9.333 g/cm^3

Thermal parameters
Overall isotropic B = 1.0

Scattering factors
Ce^0 and Co^0 [Thomas and Umeda, 1957], corrected for dispersion [Dauben and Templeton, 1955].

Scale factors (integrated intensities)
$\gamma = 0.501 \times 10^{-3}$
I/I_c (calculated) = 10.3

Additional pattern
1. Fülling, Moeller and Vogel [1942].

References

Dauben, C. H. and Templeton, D. H. (1955). Acta Crystallogr. 8, 841.

Fülling, W., Moeller, K., and Vogel, R. (1942). Z. Metallk. 34, 253.

Thomas, L.H. and Umeda, K. (1957). J. Chem. Phys. 26, 293.

Wernick, J.H. and Geller, S. (1960). Trans. AIME 218, 866.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ				2θ(°) λ = 1.540598Å
4.13	16	1	1	1		21.48
2.532	68	2	2	0		35.42
2.159	100	3	1	1		41.80
2.067	15	2	2	2		43.76
1.643	3	3	3	1		55.92
1.462	16	4	2	2		63.60
1.378	20	5	1	1	+	67.96
1.266	13	4	4	0		74.96
1.211	1	5	3	1		79.04
1.132	5	6	2	0		85.74
1.092	5	5	3	3		89.72
1.080	2	6	2	2		91.04
1.003	1	7	1	1	+	100.38
.957	6	6	4	2		107.22
.932	9	7	3	1	+	111.44
.895	2	8	0	0		118.76
.844	4	8	2	2	+	131.78
.827	6	7	5	1	+	137.36
.821	1	6	6	2		139.36
.786	1	7	5	3	+	157.04

Calculated Pattern (Integrated)

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
4.13	12	1	1	1	21.48
2.532	66	2	2	0	35.43
2.159	100	3	1	1	41.80
2.067	15	2	2	2	43.76
1.643	3	3	3	1	55.92
1.462	20	4	2	2	63.60
1.378	19	5	1	1	67.97
1.378	6	3	3	3	67.97
1.266	18	4	4	0	74.96
1.210	2	5	3	1	79.05
1.132	8	6	2	0	85.74
1.092	8	5	3	3	89.72
1.080	4	6	2	2	91.05
.957	10	6	4	2	107.21
.932	12	7	3	1	111.43
.932	6	5	5	3	111.43
.895	4	8	0	0	118.76
.844	3	6	6	0	131.78
.844	6	8	2	2	131.78
.827	14	7	5	1	137.36
.827	2	5	5	5	137.36
.821	3	6	6	2	139.36
.786	3	7	5	3	157.04
.786	1	9	1	1	157.04

Cerium cobalt, $Ce_{24}Co_{11}$

Structure
Hexagonal, $P6_3mc$ (186), Z = 2. The structure was determined by Larson and Cromer [1962].

Lattice constants:

a = 9.588 Å
c = 21.827

(published values: a = 9.587, c = 21.825 Å [ibid.]).

Density
(calculated) 7.666 g/cm^3

Thermal parameters
Isotropic [Larson and Cromer, 1962].

Scattering factors
Ce^0, Co^0 [International Tables, 1962].

Scale factors (integrated intensities)
$\gamma = 0.170 \times 10^{-3}$
I/I_c (calculated) = 3.63

References
International Tables for X-ray Crystallography III (1962), 210, 211.
Larson, A. C. and Cromer, D. T. (1962). Acta Crystallogr. 15, 1224.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ				2θ(°) λ = 1.540598Å
10.91	2	0	0	2		8.10
8.29	1	1	0	0		10.66
6.60	3	1	0	2		13.40
4.79	1	1	1	0		18.50
3.88	1	2	0	2		22.90
3.60	2	2	0	3	+	24.70
3.33	10	1	0	6		26.74
3.30	28	2	0	4		26.96
3.14	32	2	1	0		28.42
3.11	28	2	1	1		28.72
3.02	28	2	1	2		29.60
3.01	23	2	0	5		29.66
2.919	60	1	0	7		30.60
2.899	12	1	1	6		30.82
2.882	19	2	1	3		31.00
2.768	22	3	0	0		32.32
2.745	8	3	0	1		32.60
2.736	22	2	0	6		32.70
2.720	100	2	1	4	+	32.90
2.587	63	3	0	3	+	34.64
2.548	22	2	1	5		35.20
2.493	56	2	0	7		36.00
2.396	56	2	2	0		37.50
2.377	5	2	1	6		37.82
2.338	4	3	0	5		38.48
2.280	18	2	0	8		39.50
2.253	1	3	1	2		39.98
2.212	2	2	1	7		40.76
2.203	4	3	0	6		40.94
2.196	3	3	1	3		41.06
2.122	8	3	1	4		42.58
2.111	2	1	0	10		42.80
2.094	2	2	0	9		43.16
2.066	3	4	0	1		43.78
2.059	4	2	1	8		43.94
2.039	1	4	0	2		44.40
1.996	1	4	0	3		45.40
1.946	2	3	1	6		46.64
1.940	3	4	0	4	+	46.78
1.932	2	2	0	10	+	47.00
1.919	3	2	1	9		47.34
1.905	1	3	2	0		47.70
1.876	3	3	2	2	+	48.48
1.843	1	3	2	3		49.42
1.824	2	3	0	9		49.96
1.812	1	4	1	0		50.32
1.800	5	2	2	8	+	50.66
1.798	6	3	2	4		50.72
1.791	6	2	0	11	+	50.96
1.777	2	1	0	12		51.38
1.758	9	4	1	3	+	51.96
1.746	1	3	2	5		52.36
1.728	5	4	0	7		52.94
1.701	1	1	1	12		53.86
1.687	2	3	2	6		54.32
1.677	1	2	1	11		54.68
1.673	1	4	1	5		54.82
1.666	4	2	0	12		55.08
1.661	5	5	0	0		55.26
1.656	5	5	0	1		55.44
1.652	4	4	0	8		55.58
1.646	2	1	0	13		55.82
1.642	4	5	0	2		55.96
1.625	27	3	2	7		56.58
1.621	18	5	0	3	+	56.74
1.613	25	3	0	11		57.06
1.598	17	3	3	0		57.64
1.589	17	5	0	4		58.00
1.577	1	4	0	9		58.48
1.562	3	3	2	8		59.10
1.559	5	0	0	14		59.22
1.555	4	2	0	13		59.38
1.552	5	5	0	5		59.50
1.532	1	1	0	14		60.36
1.520	1	3	0	12		60.90

d(Å)	I	hkℓ				2θ(°) λ = 1.540598Å
1.511	1	5	0	6		61.32
1.504	1	4	0	10		61.60
1.477	1	5	1	2		62.86
1.463	1	3	3	6		63.54
1.449	1	2	2	12		64.24
1.441	1	4	2	6		64.64
1.438	2	5	1	4		64.76
1.435	3	3	2	10	+	64.92
1.427	1	3	1	12		65.32
1.379	3	3	3	8	+	67.92
1.375	2	3	2	11		68.14
1.373	2	2	0	15		68.24
1.370	1	5	0	9		68.42
1.365	1	4	3	0		68.70
1.359	3	6	0	3	+	69.04
1.345	3	5	1	7		69.86
1.338	5	4	1	11		70.30
1.330	2	5	2	0		70.80
1.324	4	4	3	4		71.14
1.320	3	2	1	15	+	71.38
1.316	2	3	2	12		71.68
1.308	7	5	2	3	+	72.16
1.274	1	4	2	10		74.40
1.272	1	5	2	5		74.54
1.260	2	3	2	13		75.40
1.251	1	4	3	7		76.04
1.249	1	5	2	6		76.18
1.206	2	3	2	14		79.36
1.192	1	5	1	11		80.50
1.164	1	2	0	18		82.86
1.159	3	5	3	4		83.30
1.156	3	3	2	15		83.54
1.153	2	5	1	12		83.80
1.151	1	6	2	0		83.98
1.150	2	6	2	1		84.12
1.137	1	6	2	3		85.28
1.135	3	6	0	11		85.48
1.131	4	2	1	18		85.84
1.128	3	5	3	6		86.16
1.127	4	6	2	4		86.26
1.116	2	3	3	14	+	87.30
1.113	2	6	2	5		87.56
1.109	5	5	3	7	+	88.02
1.105	5	5	2	11		88.44
1.100	3	7	1	0		88.92
1.095	1	5	0	15		89.46
1.088	2	5	3	8		90.16
1.079	1	2	1	19		91.12
1.042	1	5	3	10		95.32

Calculated Pattern (Integrated)

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
10.91	1	0	0	2	8.09
8.30	1	1	0	0	10.65
6.61	2	1	0	2	13.39
4.79	1	1	1	0	18.49
3.88	1	2	0	2	22.90
3.61	1	2	0	3	24.67
3.60	1	1	1	4	24.70
3.33	9	1	0	6	26.73
3.30	28	2	0	4	26.96
3.14	32	2	1	0	28.42
3.11	28	2	1	1	28.71
3.02	27	2	1	2	29.59
3.01	7	2	0	5	29.67
2.919	62	1	0	7	30.60
2.898	10	1	1	6	30.83
2.882	19	2	1	3	31.01
2.768	23	3	0	0	32.32
2.746	4	3	0	1	32.58
2.736	16	2	0	6	32.70
2.728	12	0	0	8	32.80
2.721	100	2	1	4	32.90
2.592	1	1	0	8	34.58
2.587	70	3	0	3	34.65
2.548	24	2	1	5	35.19
2.493	63	2	0	7	35.99
2.397	65	2	2	0	37.49
2.376	4	2	1	6	37.83
2.338	4	3	0	5	38.48
2.280	21	2	0	8	39.49
2.253	1	3	1	2	39.98
2.212	2	2	1	7	40.76
2.203	5	3	0	6	40.94
2.196	2	3	1	3	41.08
2.122	10	3	1	4	42.58
2.111	2	1	0	10	42.80
2.094	2	2	0	9	43.16
2.067	3	4	0	1	43.77
2.059	4	2	1	8	43.94
2.039	1	4	0	2	44.39
1.996	1	4	0	3	45.40
1.946	2	3	1	6	46.64
1.943	2	3	0	8	46.71
1.940	2	4	0	4	46.78
1.932	2	2	0	10	47.00
1.930	1	1	0	11	47.05
1.919	4	2	1	9	47.33
1.905	2	3	2	0	47.70
1.877	3	3	2	2	48.47
1.875	1	4	0	5	48.52
1.843	1	3	2	3	49.42

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
1.824	3	3	0	9	49.96
1.812	1	4	1	0	50.32
1.806	1	4	1	1	50.50
1.803	1	4	0	6	50.58
1.801	4	2	2	8	50.65
1.799	5	3	2	4	50.72
1.792	3	2	1	10	50.92
1.790	5	2	0	11	50.97
1.777	2	1	0	12	51.38
1.760	3	3	1	8	51.92
1.758	10	4	1	3	51.97
1.746	1	3	2	5	52.36
1.728	7	4	0	7	52.95
1.701	1	1	1	12	53.87
1.688	3	3	2	6	54.32
1.677	1	2	1	11	54.68
1.674	1	4	1	5	54.81
1.666	5	2	0	12	55.08
1.661	4	5	0	0	55.27
1.656	4	5	0	1	55.44
1.652	3	4	0	8	55.58
1.646	2	1	0	13	55.82
1.642	3	5	0	2	55.96
1.626	37	3	2	7	56.57
1.622	2	4	1	6	56.71
1.619	3	5	0	3	56.82
1.613	32	3	0	11	57.06
1.598	22	3	3	0	57.64
1.589	22	5	0	4	58.01
1.577	1	4	0	9	58.48
1.562	2	3	2	8	59.10
1.559	6	0	0	14	59.22
1.557	2	2	0	13	59.32
1.552	5	5	0	5	59.51
1.532	2	1	0	14	60.36
1.520	1	3	0	12	60.90
1.511	2	5	0	6	61.31
1.504	1	4	0	10	61.61
1.478	1	5	1	2	62.84
1.463	1	3	3	6	63.54
1.449	1	2	2	12	64.23
1.441	1	4	2	6	64.63
1.439	2	5	1	4	64.75
1.435	2	3	2	10	64.92
1.433	1	1	0	15	65.02
1.427	1	3	1	12	65.32
1.402	1	4	2	7	66.67
1.379	4	3	3	8	67.92
1.374	1	3	2	11	68.19
1.373	1	2	0	15	68.24

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
1.370	1	5	0	9	68.41
1.365	1	4	3	0	68.71
1.360	3	6	0	3	69.03
1.358	2	3	0	14	69.09
1.345	4	5	1	7	69.86
1.338	7	4	1	11	70.30
1.330	2	5	2	0	70.81
1.324	5	4	3	4	71.14
1.322	1	5	0	10	71.30
1.320	2	2	1	15	71.39
1.316	2	3	2	12	71.68
1.309	3	5	1	8	72.12
1.308	7	5	2	3	72.16
1.307	4	2	2	14	72.23
1.303	1	4	3	5	72.49
1.296	1	2	0	16	72.93
1.278	1	4	3	6	74.13
1.274	1	4	2	10	74.40
1.272	1	5	2	5	74.55
1.260	3	3	2	13	75.40
1.250	1	4	3	7	76.05
1.249	1	5	2	6	76.17
1.207	3	3	2	14	79.35
1.192	1	5	1	11	80.50
1.164	1	2	0	18	82.87
1.159	4	5	3	4	83.30
1.156	3	3	2	15	83.54
1.153	2	5	1	12	83.82
1.151	1	6	2	0	83.97
1.150	2	6	2	1	84.12
1.137	2	6	2	3	85.26
1.135	4	6	0	11	85.47
1.131	5	2	1	18	85.84
1.128	2	5	3	6	86.16
1.127	7	6	2	4	86.27
1.116	4	3	3	14	87.30
1.115	1	5	1	13	87.39
1.113	1	6	2	5	87.55
1.109	2	3	2	16	87.98
1.109	2	7	0	7	88.02
1.109	6	5	3	7	88.02
1.107	1	2	0	19	88.17
1.105	7	5	2	11	88.43
1.100	6	7	1	0	88.92
1.094	1	5	0	15	89.47
1.088	3	5	3	8	90.16
1.079	2	2	1	19	91.13
1.042	1	5	3	10	95.31
1.042	1	5	1	15	95.40

Cerium gallium, $CeGa_2$

Structure
Hexagonal, P6/mmm(191), Z=1, isostructural with AlB_2 [Laves, 1943].

Lattice constants: Haszko [1961]

$a = 4.32\text{Å}$
$c = 4.34$

Density
(calculated) 6.62 g/cm^3

Thermal parameters
Overall isotropic B = 1.0

Scattering factors
Ce^0 and Ga^0 [Thomas and Umeda, 1957], corrected for dispersion [Dauben and Templeton, 1955].

Scale factors (integrated intensities)
$\gamma = 0.388 \times 10^{-3}$
I/I_c (calculated = 12.8

References
Dauben, C. H. and Templeton, D. H. (1955). Acta Crystallogr. 8, 841.
Haszko, S. E. (1961). Trans. AIME 221, 201.
Laves, F. (1943). Naturwissenschaften 31, 145.
Thomas, L.H. and Umeda, K. (1957). J. Chem. Phys. 26, 293.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.74	13	1 0 0	23.76
2.834	100	1 0 1	31.54
2.170	14	0 0 2	41.58
2.160	37	1 1 0	41.78
1.877	3	1 0 2	48.46
1.871	2	2 0 0	48.62
1.718	17	2 0 1	53.28
1.531	18	1 1 2	60.42
1.417	1	2 0 2	65.86
1.414	1	2 1 0	66.02
1.349	6	1 0 3	69.62
1.345	12	2 1 1	69.90
1.247	3	3 0 0	76.30
1.185	1	2 1 2	81.12
1.144	3	2 0 3	84.62
1.085	1	0 0 4	90.46
1.081	4	3 0 2	90.86
1.080	3	2 2 0	91.00
1.011	3	2 1 3	99.24
1.009	4	3 1 1	99.52
.970	2	1 1 4	105.22
.967	3	2 2 2	105.62
.914	1	4 0 1	114.80
.846	1	1 0 5	131.30
.843	3	3 1 3	132.00
.842	2	3 2 1	132.38
.819	2	3 0 4	140.46
.816	3	4 1 0	141.30
.787	1	2 0 5	156.10
.785	2	4 0 3	157.46

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
3.74	11	1	0	0	23.76
2.834	100	1	0	1	31.55
2.170	13	0	0	2	41.58
2.160	38	1	1	0	41.79
1.877	3	1	0	2	48.46
1.871	2	2	0	0	48.63
1.718	20	2	0	1	53.28
1.531	22	1	1	2	60.42
1.417	1	2	0	2	65.87
1.414	1	2	1	0	66.01
1.349	8	1	0	3	69.62
1.344	15	2	1	1	69.91
1.247	5	3	0	0	76.29
1.185	1	2	1	2	81.11
1.144	4	2	0	3	84.62
1.085	1	0	0	4	90.46
1.081	6	3	0	2	90.86
1.080	3	2	2	0	91.00
1.011	6	2	1	3	99.24
1.009	6	3	1	1	99.51
.970	5	1	1	4	105.21
.967	5	2	2	2	105.63
.936	1	3	1	2	110.75
.914	3	4	0	1	114.81
.861	1	2	1	4	126.98
.846	3	1	0	5	131.29
.843	6	3	1	3	132.01
.842	6	3	2	1	132.37
.819	6	3	0	4	140.46
.816	6	4	1	0	141.31
.798	1	3	2	2	149.65
.787	5	2	0	5	156.10
.785	5	4	0	3	157.46

Cerium magnesium, $CeMg_3$

Structure
Cubic, face centered, Z=4. [Rossi and Iandelli, 1934]. Their atomic positions indicate Fm3m; other references include Fd3m as a possibility.

Lattice constant: [Vogel and Heumann, 1947]

$a = 7.438$ Å

Density
(calculated) 3.439 g/cm^3

Thermal parameters
Overall isotropic B = 1.0

Scattering factors
Ce^0, Mg^0 [International Tables, 1962].

Atom positions
Rossi and Iandelli [1934].

Scale factors (integrated intensities)
$\gamma = 0.716 \times 10^{-3}$
I/I_c (calculated) = 10.8

References

International Tables for X-ray Crystallography III (1962), 202, 211.

Rossi, A. and Iandelli, A. (1934). Atti Accad. Naz. Lincei Cl. Sci. Fis. Mat. Natur. Rend. Ser. 6, V.19, 415.

Vogel, R. and Heumann, Th. (1947). Z. Metallk. 38, 1 (1947).

Calculated Pattern (Peak heights)					
d(Å)	I	h	k	ℓ	2θ(°) λ = 1.540598Å
4.30	75	1	1	1	20.66
3.72	38	2	0	0	23.92
2.63	100	2	2	0	34.06
2.243	33	3	1	1	40.18
2.148	9	2	2	2	42.04
1.860	15	4	0	0	48.94
1.706	11	3	3	1	53.68
1.663	10	4	2	0	55.18
1.518	25	4	2	2	60.98
1.431	7	5	1	1 +	65.12
1.315	6	4	4	0	71.72
1.257	6	5	3	1	75.56
1.240	3	4	4	2 +	76.84
1.176	7	6	2	0	81.84
1.134	2	5	3	3	85.54
1.121	2	6	2	2	86.78
1.074	2	4	4	4	91.70
1.041	3	7	1	1 +	95.40
1.032	1	6	4	0	96.62
.994	7	6	4	2	101.60
.968	3	7	3	1 +	105.40
.930	1	8	0	0	111.90
.909	1	7	3	3	115.92
.902	2	8	2	0 +	117.30
.877	4	8	2	2 +	122.98
.859	2	7	5	1 +	127.50
.853	1	6	6	2	129.06
.832	3	8	4	0	135.72
.816	3	7	5	3 +	141.30
.812	2	8	4	2	143.30
.793	3	6	6	4	152.58

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
4.29	66	1	1	1	20.67
3.72	35	2	0	0	23.91
2.63	100	2	2	0	34.07
2.243	34	3	1	1	40.18
2.147	10	2	2	2	42.05
1.860	16	4	0	0	48.94
1.706	14	3	3	1	53.67
1.663	12	4	2	0	55.18
1.518	31	4	2	2	60.98
1.431	7	5	1	1	65.11
1.431	2	3	3	3	65.11
1.315	9	4	4	0	71.72
1.257	9	5	3	1	75.57
1.240	1	6	0	0	76.83
1.240	4	4	4	2	76.83
1.176	11	6	2	0	81.84
1.134	3	5	3	3	85.55
1.121	3	6	2	2	86.78
1.074	3	4	4	4	91.70
1.042	2	5	5	1	95.39
1.042	2	7	1	1	95.39
1.031	2	6	4	0	96.63
.994	13	6	4	2	101.61
.968	4	7	3	1	105.40
.968	2	5	5	3	105.40
.930	2	8	0	0	111.89
.909	2	7	3	3	115.92
.902	2	8	2	0	117.30
.902	2	6	4	4	117.30
.877	3	6	6	0	122.99
.877	6	8	2	2	122.99
.859	4	7	5	1	127.50
.859	1	5	5	5	127.50
.853	2	6	6	2	129.07
.832	7	8	4	0	135.73
.816	6	7	5	3	141.30
.816	3	9	1	1	141.30
.812	6	8	4	2	143.31
.793	10	6	6	4	152.58

Cerium nickel, $CeNi_2$

Structure
Cubic, Fd3m(227), Z=8, C15 type, isostructural with Cu_2Mg [Fülling et al., 1942].

Lattice constant: [Wernick and Geller, 1960]

a = 7.202(5)Å

Density
(calculated) 9.158 g/cm^3

Thermal parameters
Overall isotropic B = 1.0

Scattering factors
Ce^0 and Ni^0 [Thomas and Umeda, 1957], corrected for dispersion [Dauben and Templeton, 1955].

Scale factors (integrated intensities)
$\gamma = 0.774 \times 10^{-3}$
I/I_c (calculated) = 10.1

Additional patterns
1. Fülling, Moeller, and Vogel [1942].
2. Nowotny [1942].

References

Dauben, C. H. and Templeton, D. H. (1955). Acta Crystallogr. 8, 841.

Fülling W., Moeller, K., and Vogel, R. (1942). Z. Metallk. 34, 253.

Nowotny, H. (1942). Z. Metallk. 34 #11, 247.

Thomas, L.H. and Umeda, K. (1957). J. Chem. Phys. 26, 293.

Wernick, J.H. and Geller, S. (1960). Trans. AIME 218, 866.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ				2θ(°) λ = 1.540598Å
4.16	16	1	1	1		21.36
2.546	72	2	2	0		35.22
2.171	100	3	1	1		41.56
2.079	14	2	2	2		43.50
1.652	3	3	3	1		55.58
1.470	17	4	2	2		63.20
1.386	20	5	1	1	+	67.52
1.273	13	4	4	0		74.46
1.217	2	5	3	1		78.50
1.139	5	6	2	0		85.14
1.098	5	5	3	3		89.08
1.086	2	6	2	2		90.38
1.009	1	7	1	1	+	99.60
.962	6	6	4	2		106.34
.938	8	7	3	1	+	110.48
.900	2	8	0	0		117.66
.849	4	8	2	2	+	130.34
.832	6	7	5	1	+	135.72
.826	1	6	6	2		137.64
.791	1	7	5	3	+	154.02

Calculated Pattern (Integrated)

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
4.16	13	1	1	1	21.35
2.546	67	2	2	0	35.22
2.171	100	3	1	1	41.55
2.079	15	2	2	2	43.49
1.652	3	3	3	1	55.58
1.470	21	4	2	2	63.20
1.386	19	5	1	1	67.53
1.386	6	3	3	3	67.53
1.273	18	4	4	0	74.46
1.217	3	5	3	1	78.51
1.139	8	6	2	0	85.13
1.098	8	5	3	3	89.07
1.086	3	6	2	2	90.38
1.008	1	7	1	1	99.60
1.008	1	5	5	1	99.60
.962	11	6	4	2	106.33
.938	11	7	3	1	110.48
.938	6	5	5	3	110.48
.900	3	8	0	0	117.66
.880	1	7	3	3	122.20
.849	3	6	6	0	130.34
.849	6	8	2	2	130.34
.832	13	7	5	1	135.72
.832	2	5	5	5	135.72
.826	2	6	6	2	137.63
.805	1	8	4	0	146.13
.791	3	7	5	3	154.02
.791	2	9	1	1	154.02

Cerium thallium, CeTl

Structure
Cubic, Pm3m (221), Z = 1, CsCl type [Bruzzone and Ferro Ruggiero, 1962].

Lattice constant: [ibid.]

$a = 3.893$ Å

Density
(calculated) 9.695 g/cm^3

Thermal parameters
Overall isotropic B = 1.0

Scattering factors
Ce^0, Tl^0 [International Tables, 1962].

Scale factors (integrated intensities)
$\gamma = 1.90 \times 10^{-3}$
I/I_c (calculated) = 32.3

References
International Tables for X-ray Crystallography III (1962), 211, 212.
Bruzzone, G. and Ferro Ruggiero, A. (1962). Atti Accad. Naz. Lincei Cl. Sci. Fis. Mat. Natur. Rend. 33, 465.

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.89	4	1 0 0	22.82
2.753	100	1 1 0	32.50
2.248	1	1 1 1	40.08
1.947	17	2 0 0	46.62
1.741	2	2 1 0	52.52
1.589	34	2 1 1	57.98
1.376	10	2 2 0	68.06
1.231	13	3 1 0	77.47
1.124	3	2 2 2	86.54
1.040	15	3 2 1	95.52
.973	2	4 0 0	104.65
.918	3	3 3 0	114.17
.918	6	4 1 1	114.17
.871	7	4 2 0	124.48
.830	8	3 3 2	136.28
.795	11	4 2 2	151.56

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.89	4	1 0 0	22.82
2.753	100	1 1 0	32.50
2.248	1	1 1 1	40.08
1.947	15	2 0 0	46.62
1.741	1	2 1 0	52.52
1.589	27	2 1 1	57.98
1.376	7	2 2 0	68.06
1.231	8	3 1 0	77.46
1.124	2	2 2 2	86.54
1.040	8	3 2 1	95.52
.973	1	4 0 0	104.64
.918	4	4 1 1 +	114.18
.870	3	4 2 0	124.48
.830	3	3 3 2	136.28
.795	3	4 2 2	151.56

Cerium thallium, $CeTl_3$

Structure
Cubic, Pm3m (221), Z = 1, $AuCu_3$ type [Bruzzone and Ferro Ruggiero, 1962].

Lattice constant: [ibid.]

$a = 4.767$ Å

Density
(calculated) 11.55 g/cm^3

Thermal parameters
Overall isotropic B = 1.0

Scattering factors
Ce^0, Tl^0 [International Tables, 1962].

Scale factors (integrated intensities)
$\gamma = 1.66 \times 10^{-3}$
I/I_c (calculated) = 25.4

References
International Tables for X-ray Crystallography III (1962), 211, 212.
Bruzzone, G. and Ferro Ruggiero, A. (1962). Atti Accad. Naz. Lincei Cl. Sci. Fis. Mat. Natur. Rend. 33, 465.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.77	2	1 0 0	18.60
3.37	2	1 1 0	26.42
2.753	100	1 1 1	32.50
2.383	47	2 0 0	37.72
2.132	1	2 1 0	42.36
1.685	26	2 2 0	54.40
1.437	27	3 1 1	64.82
1.376	7	2 2 2	68.08
1.192	3	4 0 0	80.54
1.094	8	3 3 1	89.56
1.066	7	4 2 0	92.54
.973	5	4 2 2	104.68
.917	6	5 1 1 +	114.20
.843	2	4 4 0	132.16
.806	9	5 3 1	145.88
.795	6	4 4 2 +	151.64

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.77	2	1 0 0	18.60
3.37	2	1 1 0	26.42
2.752	100	1 1 1	32.51
2.384	49	2 0 0	37.71
2.132	1	2 1 0	42.36
1.946	1	2 1 1	46.63
1.685	32	2 2 0	54.39
1.437	35	3 1 1	64.81
1.376	10	2 2 2	68.08
1.192	4	4 0 0	80.54
1.094	13	3 3 1	89.55
1.066	12	4 2 0	92.55
.973	10	4 2 2	104.68
.917	10	5 1 1	114.21
.917	3	3 3 3	114.21
.843	6	4 4 0	132.15
.806	29	5 3 1	145.87
.795	17	4 4 2	151.64
.795	4	6 0 0	151.64

Cerium thallium, Ce_3Tl

Structure
Cubic, Pm3m (221), Z = 1, $AuCu_3$ type [Jeitschko et al., 1964].

Lattice constant: [ibid.]

$a = 5.011$ Å

Density
(calculated) 8.245 g/cm^3

Thermal parameters
Overall isotropic B = 1.0

Scattering factors
Ce^0, Tl^0 [International Tables, 1962].

Scale factors (integrated intensities)
$\gamma = 2.09 \times 10^{-3}$
I/I_c (calculated) = 37.2

References

International Tables for X-ray Crystallography III (1962), 211, 212.
Jeitschko, W., Nowotny, H., and Benesovsky, F. (1964). Monatsh. Chem. 95, 1040.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ				2θ(°) λ = 1.540598Å
5.01	34	1	0	0		17.68
3.54	27	1	1	0		25.12
2.893	100	1	1	1		30.88
2.505	46	2	0	0		35.82
2.241	13	2	1	0		40.20
2.046	10	2	1	1		44.24
1.772	27	2	2	0		51.54
1.670	5	2	2	1	+	54.92
1.584	3	3	1	0		58.18
1.511	27	3	1	1		61.30
1.446	7	2	2	2		64.36
1.390	2	3	2	0		67.32
1.339	3	3	2	1		70.22
1.253	3	4	0	0		75.88
1.215	2	4	1	0	+	78.66
1.181	1	4	1	1	+	81.42
1.150	8	3	3	1		84.14
1.120	7	4	2	0		86.86
1.094	1	4	2	1		89.56
1.023	5	4	2	2		97.72
.983	1	4	3	1	+	103.22
.964	6	5	1	1	+	106.02
.930	1	4	3	2	+	111.76
.915	1	5	2	1		114.70
.886	2	4	4	0		120.82
.872	1	5	2	2	+	124.02
.859	1	5	3	0	+	127.36
.847	7	5	3	1		130.86
.835	4	4	4	2	+	134.54
.813	1	5	3	2	+	142.74
.792	4	6	2	0		152.92
.783	2	6	2	1	+	159.66

Calculated Pattern (Integrated)					
d(Å)	I	h	k	ℓ	2θ(°) λ = 1.540598Å
5.01	30	1	0	0	17.69
3.54	26	1	1	0	25.11
2.893	100	1	1	1	30.88
2.505	50	2	0	0	35.81
2.241	14	2	1	0	40.21
2.046	11	2	1	1	44.24
1.772	33	2	2	0	51.54
1.670	1	3	0	0	54.92
1.670	5	2	2	1	54.92
1.585	5	3	1	0	58.17
1.511	37	3	1	1	61.31
1.447	10	2	2	2	64.35
1.390	3	3	2	0	67.32
1.339	5	3	2	1	70.22
1.253	4	4	0	0	75.89
1.215	2	4	1	0	78.66
1.215	2	3	2	2	78.66
1.181	1	3	3	0	81.41
1.181	2	4	1	1	81.41
1.150	13	3	3	1	84.14
1.120	12	4	2	0	86.86
1.093	2	4	2	1	89.57
1.068	1	3	3	2	92.28
1.023	9	4	2	2	97.72
1.002	1	4	3	0	100.46
.983	2	4	3	1	103.23
.983	1	5	1	0	103.23
.964	9	5	1	1	106.02
.964	3	3	3	3	106.02
.931	1	5	2	0	111.75
.931	2	4	3	2	111.75
.915	2	5	2	1	114.70
.886	4	4	4	0	120.82
.872	1	4	4	1	124.03
.872	1	5	2	2	124.03
.859	1	5	3	0	127.36
.859	1	4	3	3	127.36
.847	18	5	3	1	130.85
.835	2	6	0	0	134.54
.835	10	4	4	2	134.54
.824	1	6	1	0	138.47
.813	2	5	3	2	142.74
.813	1	6	1	1	142.74
.792	15	6	2	0	152.93
.793	2	5	4	0	159.67
.783	4	6	2	1	159.67
.783	2	4	4	3	159.67

Cobalt dysprosium, Co_2Dy

Structure
Cubic, Fd3m(227), Z=8, C15 type, isostructural with Cu_2Mg [Wernick and Geller, 1960].

Lattice constant: [ibid.]

a = 7.187(5)Å

Density
(calculated) 10.033 g/cm^3

Thermal parameters
Overall isotropic B = 1.0

Scattering factors
Co^0 and Dy^0 [Thomas and Umeda, 1957], corrected for dispersion [Dauben and Templeton, 1955].

Scale factors (integrated intensities)
$\gamma = 0.510 \times 10^{-3}$
I/I_c (calculated) = 9.35

References

Dauben, C. H. and Templeton, D. H. (1955). Acta Crystallogr. 8, 841.

Thomas, L.H. and Umeda, K. (1957). J. Chem. Phys. 26, 293.

Wernick, J.H. and Geller, S. (1960). Trans. AIME 218, 866.

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.15	13	1 1 1	21.40
2.541	66	2 2 0	35.29
2.167	100	3 1 1	41.65
2.075	16	2 2 2	43.59
1.649	3	3 3 1	55.70
1.467	19	4 2 2	63.35
1.383	19	5 1 1	67.69
1.383	6	3 3 3	67.69
1.270	17	4 4 0	74.64
1.215	2	5 3 1	78.70
1.136	7	6 2 0	85.35
1.096	8	5 3 3	89.31
1.083	4	6 2 2	90.62
.960	9	6 4 2	106.65
.936	11	7 3 1	110.83
.936	5	5 5 3	110.83
.898	3	8 0 0	118.06
.847	2	6 6 0	130.86
.847	5	8 2 2	130.86
.830	12	7 5 1	136.31
.830	2	5 5 5	136.31
.824	3	6 6 2	138.25
.789	2	7 5 3	155.08
.789	1	9 1 1	155.08

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ		2θ(°) λ = 1.540598Å
4.15	16	1 1 1		21.40
2.541	70	2 2 0		35.30
2.167	100	3 1 1		41.64
2.075	15	2 2 2		43.58
1.649	2	3 3 1		55.70
1.467	16	4 2 2		63.34
1.383	19	5 1 1	+	67.68
1.271	13	4 4 0		74.64
1.215	1	5 3 1		78.70
1.136	5	6 2 0		85.36
1.096	5	5 3 3		89.30
1.084	2	6 2 2		90.62
.960	5	6 4 2		106.66
.936	8	7 3 1	+	110.82
.898	2	8 0 0		118.06
.847	3	8 2 2	+	130.86
.830	5	7 5 1	+	136.32
.824	1	6 6 2		138.26

Cobalt erbium, Co_2Er

Structure
Cubic, Fd3m(227), Z=8, C15 type, isostructural with Cu_2Mg [Wernick and Geller, 1960].

Lattice constant: [ibid.]

$a = 7.144(5)\text{Å}$

Density
(calculated) 10.388 g/cm^3

Thermal parameters
Overall isotropic B = 1.0

Scattering factors
Co^0 and Er^0 [Thomas and Umeda, 1957], corrected for dispersion [Dauben and Templeton, 1955].

Scale factors (integrated intensities)
$\gamma = 0.762 \times 10^{-3}$
I/I_c (calculated) = 9.76

References
Dauben, C. H. and Templeton, D. H. (1955). Acta Crystallogr. 8, 841.
Thomas, L.H. and Umeda, K. (1957). J. Chem. Phys. 26, 293.
Wernick, J.H. and Geller, S. (1960). Trans. AIME 218, 866.

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.12	15	1 1 1	21.53
2.526	68	2 2 0	35.51
2.154	100	3 1 1	41.91
2.062	15	2 2 2	43.87
1.639	3	3 3 1	56.07
1.458	20	4 2 2	63.77
1.375	19	5 1 1	68.15
1.375	6	3 3 3	68.15
1.263	17	4 4 0	75.17
1.208	2	5 3 1	79.27
1.130	7	6 2 0	85.99
1.089	8	5 3 3	89.99
1.077	4	6 2 2	91.32
.955	9	6 4 2	107.59
.930	11	7 3 1	111.83
.930	5	5 5 3	111.83
.893	4	8 0 0	119.22
.842	2	6 6 0	132.39
.842	5	8 2 2	132.39
.825	13	7 5 1	138.07
.825	2	5 5 5	138.07
.819	3	6 6 2	140.10
.784	2	7 5 3	158.43
.784	1	9 1 1	158.43

Calculated Pattern (Peak heights)

d$_c$(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.12	19	1 1 1	21.54
2.525	74	2 2 0	35.52
2.154	100	3 1 1	41.90
2.063	15	2 2 2	43.86
1.639	3	3 3 1	56.06
1.458	16	4 2 2	63.78
1.375	19	5 1 1 +	68.14
1.263	13	4 4 0	75.18
1.207	1	5 3 1	79.28
1.129	5	6 2 0	86.00
1.089	5	5 3 3	90.00
1.077	2	6 2 2	91.32
.955	5	6 4 2	107.58
.930	8	7 3 1 +	111.84
.893	2	8 0 0	119.22
.842	3	8 2 2 +	132.38
.825	6	7 5 1 +	138.06
.819	1	6 6 2	140.10

Cobalt erbium, Co_7Er_2

Structure
Hexagonal, $R\bar{3}m(166)$, Z = 6. The structure was determined by Ostertag [1967].

Lattice constants: [ibid.]

a = 4.973Å
c = 36.11

Density
(measured) 9.620 g/cm^3 [ibid.]
(calculated) 9.624 g/cm^3

Thermal parameters
Isotropic [Ostertag, op. cit.]

Scattering factors
Co^0, Er^0 [International Tables, 1962].

Scale factors (integrated intensities)
$\gamma = 0.467 \times 10^{-3}$
I/I_c (calculated) 6.70

References
International Tables for X-ray Crystallography III (1962), 204, 212.
Ostertag, W. (1967). J. Less-Common Metals, 13, 385.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
12.04	5	0 0 3	7.34
6.02	1	0 0 6	14.72
4.28	12	1 0 1	20.76
4.19	2	0 1 2	21.20
4.01	5	0 0 9	22.14
3.89	4	1 0 4	22.86
3.116	2	0 1 8	28.64
3.009	5	0 0 12	29.68
2.767	49	1 0 10	32.34
2.611	39	0 1 11	34.32
2.487	58	1 1 0	36.10
2.407	2	0 0 15	37.32
2.334	2	1 0 13	38.54
2.213	9	0 1 14	40.74
2.150	40	0 2 1	42.00
2.114	100	1 1 9	42.76
2.095	10	0 2 4	43.14
2.064	4	2 0 5	43.84
2.006	14	0 0 18	45.16
1.999	10	1 0 16	45.26
1.987	8	0 2 7	45.62
1.944	12	2 0 8	46.70
1.917	8	1 1 12	47.40
1.905	7	0 1 17	47.70
1.801	3	2 0 11	50.66
1.730	3	1 1 15	52.90
1.720	4	0 0 21	53.22
1.665	6	0 1 20	55.12
1.653	1	2 0 14	55.54
1.626	2	2 1 1	56.56
1.561	2	1 1 18	59.12
1.558	2	0 2 16	59.28
1.534	3	1 0 22	60.30
1.512	1	2 0 17	61.24
1.505	1	0 0 24	61.58
1.484	13	2 1 10	62.54
1.458	11	1 2 11	63.76
1.436	9	3 0 0	64.90
1.425	6	0 2 19	65.44
1.414	12	1 1 21	66.00
1.384	8	2 0 20	67.66
1.377	4	1 2 14	68.06
1.369	2	1 0 25	68.46
1.352	20	3 0 9+	69.48
1.296	2	3 0 12+	72.96
1.292	4	1 2 17	73.20
1.287	3	1 1 24	73.50
1.269	1	2 0 23	74.78
1.243	19	2 2 0	76.58
1.233	1	3 0 15+	77.32
1.209	4	1 2 20	79.16
1.204	2	0 0 30	79.58
1.196	1	0 1 29	80.18
1.194	1	1 3 1	80.38
1.188	1	2 2 9	80.88
1.178	3	1 1 27	81.68
1.167	2	2 0 26+	82.60
1.156	2	2 1 22	83.60
1.149	1	2 2 12	84.20
1.134	5	1 3 10	85.58
1.124	3	1 0 31	86.48
1.122	5	3 1 11	86.68
1.106	2	0 2 28	88.26
1.102	6	0 3 21+	88.70
1.083	6	1 1 30+	90.62
1.080	4	2 1 25	90.92
1.076	4	4 0 1	91.42
1.057	8	2 2 18	93.60
1.047	1	0 4 8	94.70
1.041	2	3 1 17	95.44

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.039	2	0 3 24+	95.74
1.025	3	0 2 31	97.50
1.007	4	2 2 21	99.74
1.003	2	0 0 36	100.34
.9995	1	2 0 32	100.82
.9962	3	3 1 20	101.30
.9890	1	1 2 29	102.32
.9786	1	3 0 27+	103.84
.9658	1	1 3 22	105.80
.9584	1	2 2 24	106.98
.9530	5	3 2 10+	107.86
.9473	3	2 1 31	108.82
.9461	4	2 3 11	109.02
.9398	6	4 1 0	110.10
.9368	3	4 0 19	110.52
.9304	3	2 0 35+	111.78
.9247	3	0 4 20	112.82
.9224	6	3 0 30+	113.26
.9205	3	1 3 25	113.66
.9150	14	1 4 9+	114.66
.9106	1	2 2 27	115.54
.8971	2	1 4 12+	118.34
.8959	1	2 3 17	118.60
.8895	1	2 1 34+	120.00
.8835	1	1 0 40	121.34
.8755	1	1 4 15+	123.26
.8677	1	1 1 39	125.20
.8667	3	2 3 20	125.42
.8648	5	2 2 30	125.94
.8629	3	0 1 41	126.48
.8509	1	0 4 26+	129.70
.8465	1	3 2 22	131.00
.8378	2	0 5 10	133.68
.8370	1	2 1 37	133.92
.8339	3	1 3 31	134.94
.8331	2	5 0 11	135.20
.8288	3	3 3 0	136.68
.8265	2	4 0 28	137.44
.8247	8	4 1 21+	138.16
.8203	1	3 1 32	139.80
.8170	1	5 0 14	141.08
.8155	2	3 2 25+	141.70
.8137	6	2 4 1	142.42
.8126	3	1 1 42	142.90
.8117	10	3 3 9	143.24
.8106	2	2 4 4	143.70
.8088	1	4 2 5	144.52
.8062	1	0 1 44	145.68
.8040	1	2 4 7	146.72
.8010	2	4 2 8	148.18

Calculated Pattern (Integrated)			
d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
12.04	4	0 0 3	7.34
6.02	1	0 0 6	14.71
4.28	10	1 0 1	20.75
4.19	1	0 1 2	21.19
4.01	4	0 0 9	22.14
3.89	3	1 0 4	22.86
3.116	2	0 1 8	28.63
3.009	5	0 0 12	29.66
2.767	46	1 0 10	32.33
2.611	37	0 1 11	34.32
2.487	55	1 1 0	36.09
2.407	2	0 0 15	37.32
2.334	1	1 0 13	38.54
2.213	9	0 1 14	40.74
2.150	38	0 2 1	42.00
2.138	9	2 0 2	42.23
2.114	100	1 1 9	42.75
2.095	6	0 2 4	43.15
2.064	4	2 0 5	43.84
2.006	14	0 0 18	45.16
1.999	1	1 0 16	45.33
1.987	7	0 2 7	45.61
1.944	12	2 0 8	46.70
1.917	7	1 1 12	47.39
1.905	7	0 1 17	47.70
1.801	3	2 0 11	50.66
1.730	3	1 1 15	52.89
1.720	4	0 0 21	53.23
1.665	7	0 1 20	55.11
1.653	1	2 0 14	55.55
1.626	2	2 1 1	56.55
1.561	2	1 1 18	59.12
1.558	1	0 2 16	59.26
1.534	3	1 0 22	60.30
1.512	1	2 0 17	61.25
1.505	1	0 0 24	61.59
1.484	14	2 1 10	62.54
1.458	12	1 2 11	63.77
1.436	10	3 0 0	64.90
1.425	6	0 2 19	65.45
1.414	13	1 1 21	66.00
1.384	9	2 0 20	67.66
1.377	4	1 2 14	68.05
1.369	2	1 0 25	68.46
1.352	11	3 0 9	69.49
1.352	11	0 3 9	69.49
1.296	1	3 0 12	72.96
1.296	1	0 3 12	72.96
1.292	4	1 2 17	73.20
1.287	3	1 1 24	73.51

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.269	1	2 0 23	74.77
1.243	21	2 2 0	76.57
1.209	5	1 2 20	79.16
1.204	1	0 0 30	79.58
1.196	1	0 1 29	80.18
1.194	1	1 3 1	80.37
1.188	1	2 2 9	80.88
1.178	3	1 1 27	81.69
1.167	2	2 0 26	82.60
1.156	2	2 1 22	83.59
1.149	2	2 2 12	84.19
1.134	6	1 3 10	85.57
1.124	2	1 0 31	86.48
1.122	5	3 1 11	86.67
1.106	2	0 2 28	88.25
1.105	1	2 2 15	88.43
1.102	3	3 0 21	88.69
1.102	3	0 3 21	88.69
1.084	2	3 1 14	90.58
1.083	5	1 1 30	90.63
1.080	2	2 1 25	90.96
1.076	4	4 0 1	91.41
1.075	1	0 4 2	91.57
1.057	9	2 2 18	93.59
1.054	1	4 0 7	93.92
1.047	1	0 4 8	94.70
1.041	2	3 1 17	95.44
1.039	1	3 0 24	95.74
1.039	1	0 3 24	95.74
1.025	4	0 2 31	97.50
1.007	5	2 2 21	99.74
1.003	2	0 0 36	100.34
.9995	1	2 0 32	100.83
.9962	3	3 1 20	101.29
.9890	1	1 2 29	102.31
.9786	1	0 3 27	103.85
.9786	1	3 0 27	103.85
.9658	2	1 3 22	105.80
.9584	1	2 2 24	106.98
.9530	5	3 2 10	107.86
.9525	2	0 2 34	107.94
.9473	4	2 1 31	108.81
.9461	4	2 3 11	109.01
.9398	7	4 1 0	110.10
.9368	2	4 0 19	110.62
.9304	3	2 0 35	111.77
.9302	1	1 1 36	111.80
.9274	1	1 2 32	112.32
.9247	4	0 4 20	112.81
.9227	2	2 3 14	113.20

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
.9224	2	3 0 30	113.26
.9224	2	0 3 30	113.26
.9205	2	1 3 25	113.61
.9150	10	4 1 9	114.67
.9150	10	1 4 9	114.67
.9106	1	2 2 27	115.55
.8971	1	4 1 12	118.34
.8971	1	1 4 12	118.34
.8959	2	2 3 17	118.60
.8895	1	2 1 34	120.00
.8835	2	1 0 40	121.34
.8677	1	1 1 39	125.19
.8667	4	2 3 20	125.43
.8648	6	2 2 30	125.94
.8629	2	0 1 41	126.43
.8620	1	3 1 29	126.67
.8509	1	0 4 26	129.71
.8465	2	3 2 22	131.01
.8378	3	0 5 10	133.67
.8370	1	2 1 37	133.93
.8339	5	1 3 31	134.94
.8331	3	5 0 11	135.21
.8325	1	0 2 40	135.41
.8288	5	3 3 0	136.68
.8265	2	4 0 28	137.50
.8247	8	4 1 21	138.16
.8247	8	1 4 21	138.16
.8222	1	0 3 36	139.05
.8222	1	3 0 36	139.05
.8203	1	3 1 32	139.79
.8170	1	5 0 14	141.07
.8155	2	3 2 25	141.67
.8152	2	2 0 41	141.80
.8137	11	2 4 1	142.41
.8131	2	4 2 2	142.67
.8126	2	1 1 42	142.88
.8117	15	3 3 9	143.25
.8106	2	2 4 4	143.71
.8088	1	4 2 5	144.51
.8062	2	0 1 44	145.69
.8040	3	2 4 7	146.73
.8010	4	4 2 8	148.18
.7991	2	3 3 12	149.15
.7982	2	5 0 17	149.60
.7971	3	4 1 24	150.21
.7971	3	1 4 24	150.21
.7937	2	1 3 34	152.11
.7907	8	4 0 31	153.94
.7900	3	4 2 11	154.37
.7895	9	2 1 40	154.69

Cobalt gadolinium, $CoGd_3$

Structure
Orthorhombic, Pnma(62), Z=4, isostructural with CFe_3, type DO_{11}. The structure was determined by Strydom and Alberts [1970].

Lattice constants: [ibid.]

a = 7.05Å
b = 9.54
c = 6.32

Density
(calculated) 8.29 g/cm^3

Thermal parameters
Isotropic [Strydom and Alberts, op. cit.].

Scattering factors
Co^0, Gd^0 [Cromer and Mann, 1968].

Scale factors (integrated intensities)
$\gamma = 0.168 \times 10^{-3}$
I/I_c (calculated) 4.41

References
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Strydom, O.A.W. and Alberts, L. (1970). J. Less-Common Metals, 22, 511.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.22	1	1 1 1	21.04
3.525	1	2 0 0	25.26
3.350	18	1 2 1	26.60
3.307	13	2 1 0	26.96
3.160	9	0 0 2	28.22
3.079	15	2 0 1	28.98
2.930	35	2 1 1	30.50
2.884	38	1 0 2	31.00
2.841	100	0 3 1+	31.52
2.760	51	1 1 2	32.42
2.635	40	1 3 1+	34.00
2.587	44	2 2 1	34.66
2.468	14	1 2 2	36.38
2.385	6	0 4 0	37.70
2.361	15	2 3 0	38.08
2.284	8	2 1 2	39.42
2.203	15	3 0 1	40.94
2.146	8	3 1 1	42.08
2.136	6	1 3 2	42.16
2.127	2	1 4 1	42.44
2.110	3	2 2 2	42.82
1.975	7	2 4 0+	45.92
1.891	2	2 3 2	48.08
1.885	3	2 4 1	48.22
1.859	16	1 2 3	48.96
1.827	3	0 5 1	49.88
1.811	3	3 3 1+	50.40
1.777	1	2 1 3	51.40
1.768	1	1 5 1	51.66
1.754	3	3 2 2	52.12
1.704	14	1 3 3	53.74
1.698	16	4 0 1	53.96
1.678	5	2 5 0	54.66
1.671	4	4 1 1	54.80
1.653	1	4 2 0	55.54
1.622	24	3 3 2+	56.72
1.599	2	4 2 1	57.60
1.591	15	1 5 2+	57.92
1.580	3	0 0 4	58.36
1.569	10	3 0 3	58.82
1.542	17	4 3 0+	59.96
1.490	2	3 2 3	62.26
1.482	3	2 5 2	62.64
1.479	2	3 4 2	62.80
1.467	2	1 2 4	63.36
1.465	2	4 2 2	63.44
1.442	2	3 5 1+	64.58
1.426	1	2 1 4	65.42
1.420	1	0 6 2	65.60
1.413	1	2 6 1+	66.08
1.392	3	1 6 2	67.18
1.387	6	1 5 3+	67.50
1.380	3	2 2 4	67.84
1.362	1	5 1 1	68.88
1.341	1	3 5 2	70.10
1.332	1	0 7 1	70.64
1.322	1	5 2 1	71.26
1.317	1	0 4 4+	71.56
1.301	1	4 2 3	72.64
1.295	1	4 5 0+	73.02
1.289	2	3 6 1	73.38
1.268	1	4 5 1	74.80
1.264	1	3 2 4	75.04
1.243	4	5 2 2+	76.58
1.234	1	2 4 4+	77.28
1.232	1	1 7 2	77.38
1.212	4	3 3 4	78.92
1.199	1	1 5 4	79.94
1.198	1	4 5 2	80.02
1.194	1	5 3 2+	80.38

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.190	1	2 0 5	80.64
1.181	1	2 1 5	81.46
1.175	3	0 3 5+	81.96
1.172	3	5 0 3	82.20
1.166	1	6 1 0	82.68
1.163	2	5 1 3	82.96
1.161	4	4 6 1	83.18
1.159	2	1 3 5	83.34
1.156	2	1 8 1	83.58
1.154	1	2 2 5	83.70
1.150	1	2 5 4	84.08
1.141	1	6 2 0+	84.94
1.138	1	5 2 3	85.20
1.133	1	5 4 2	85.66
1.130	2	2 8 0	85.98
1.123	1	6 2 1	86.64
1.121	1	0 6 4	86.84
1.117	3	3 6 3+	87.24
1.112	3	2 8 1	87.68
1.107	2	1 6 4	88.20
1.103	2	4 3 4+	88.54
1.102	2	1 8 2+	88.70
1.086	2	6 3 1	90.38
1.084	1	3 2 5	90.56
1.081	1	3 5 4	90.92
1.078	1	4 7 0	91.20
1.067	1	5 5 2	92.40
1.053	1	0 0 6	94.00
1.045	1	0 9 1+	94.92
1.042	1	1 5 5	95.30
1.027	3	1 8 3+	97.20
1.010	1	2 5 5	99.46
1.001	1	6 5 0	100.70
.9985	2	5 5 3+	100.96
.9882	1	6 5 1	102.44
.9874	1	2 2 6	102.52
.9596	2	7 0 2	106.78
.9540	1	0 10 0	107.70
.9493	1	3 8 3+	108.48
.9433	1	1 8 4+	109.50
.9240	1	3 9 2	112.94
.9213	1	5 5 4	113.46
.9189	1	2 8 4	113.92
.8921	1	2 5 6	119.42
.8906	1	4 7 4+	119.88
.8781	1	0 6 6	122.64
.8749	2	5 8 2+	123.38
.8737	2	7 3 3	123.70
.8697	1	4 3 6	124.68
.8628	1	4 6 5	126.46
.8586	1	8 2 1+	127.60

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.22	1	1 1 1	21.03
3.525	1	2 0 0	25.24
3.350	23	1 2 1	26.59
3.307	16	2 1 0	26.94
3.160	12	0 0 2	28.22
3.079	20	2 0 1	28.98
2.930	46	2 1 1	30.49
2.884	48	1 0 2	30.99
2.841	100	0 3 1	31.47
2.835	57	2 2 0	31.53
2.760	69	1 1 2	32.41
2.635	42	1 3 1	34.00
2.634	14	0 2 2	34.00
2.587	61	2 2 1	34.65
2.468	19	1 2 2	36.38
2.385	9	0 4 0	37.69
2.361	21	2 3 0	38.08
2.353	4	2 0 2	38.22
2.284	11	2 1 2	39.41
2.212	2	2 3 1	40.76
2.203	20	3 0 1	40.94
2.146	11	3 1 1	42.07
2.136	3	1 3 2	42.27
2.127	2	1 4 1	42.46
2.110	4	2 2 2	42.82
2.057	1	0 1 3	43.98
1.975	6	2 4 0	45.90
1.975	5	1 1 3	45.92
1.891	2	2 3 2	48.06
1.885	3	2 4 1	48.23
1.859	24	1 2 3	48.96
1.827	4	0 5 1	49.89
1.811	3	3 3 1	50.35
1.808	2	2 0 3	50.42
1.777	1	2 1 3	51.39
1.768	1	1 5 1	51.65
1.754	4	3 2 2	52.11
1.704	20	1 3 3	53.75
1.698	19	4 0 1	53.97
1.691	1	2 2 3	54.20
1.678	8	2 5 0	54.65
1.671	3	4 1 1	54.88
1.653	1	4 2 0	55.54
1.622	24	3 3 2	56.71
1.622	13	2 5 1	56.72
1.618	2	3 4 1	56.85
1.599	1	4 2 1	57.58
1.591	15	1 5 2	57.91
1.590	10	0 6 0	57.95
1.580	3	0 0 4	58.36

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.572	1	2 3 3	58.68
1.569	14	3 0 3	58.82
1.548	1	3 1 3	59.69
1.542	8	1 0 4	59.95
1.542	14	4 3 0	59.96
1.541	5	1 4 3	59.99
1.490	3	3 2 3	62.25
1.482	5	2 5 2	62.63
1.479	1	3 4 2	62.77
1.467	3	1 2 4	63.35
1.465	1	4 2 2	63.45
1.442	2	3 5 1	64.57
1.441	1	2 4 3	64.63
1.426	2	2 1 4	65.41
1.420	1	0 6 2	65.69
1.413	1	2 6 1	66.09
1.392	4	1 6 2	67.19
1.387	2	1 3 4	67.46
1.387	6	1 5 3	67.50
1.385	4	4 3 2	67.56
1.383	1	4 4 1	67.69
1.380	3	2 2 4	67.85
1.362	1	5 1 1	68.88
1.341	2	3 5 2	70.11
1.332	2	0 7 1	70.65
1.322	2	5 2 1	71.26
1.309	1	1 7 1	72.09
1.301	1	4 2 3	72.64
1.295	1	4 5 0	73.02
1.289	3	3 6 1	73.38
1.268	2	4 5 1	74.79
1.264	1	3 2 4	75.07
1.244	1	1 0 5	76.51
1.243	5	5 2 2	76.58
1.234	1	2 4 4	77.26
1.232	1	1 7 2	77.39
1.212	7	3 3 4	78.91
1.212	1	3 5 3	78.95
1.199	1	1 5 4	79.93
1.198	1	4 5 2	80.03
1.194	1	5 3 2	80.39
1.190	1	2 0 5	80.69
1.181	2	2 1 5	81.45
1.175	1	6 0 0	81.93
1.175	4	0 3 5	81.96
1.172	1	5 0 3	82.20
1.166	1	6 1 0	82.68
1.163	3	5 1 3	82.95
1.161	5	4 6 1	83.17
1.159	1	1 3 5	83.34

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.156	1	1 8 1	83.58
1.154	1	2 2 5	83.71
1.150	1	2 5 4	84.08
1.141	1	6 2 0	84.93
1.138	1	5 2 3	85.21
1.133	1	5 4 2	85.66
1.130	2	2 8 0	85.99
1.123	1	6 2 1	86.64
1.121	1	0 6 4	86.83
1.117	4	3 6 3	87.23
1.116	1	5 5 1	87.28
1.116	1	0 8 2	87.33
1.112	4	2 8 1	87.69
1.107	2	1 6 4	88.20
1.105	1	3 7 2	88.43
1.103	2	4 3 4	88.55
1.102	2	1 8 2	88.70
1.101	1	6 0 2	88.76
1.086	2	6 3 1	90.38
1.084	1	3 2 5	90.56
1.081	2	3 5 4	90.93
1.078	1	4 7 0	91.20
1.067	1	5 5 2	92.39
1.053	1	0 0 6	93.99
1.045	1	0 9 1	94.93
1.042	1	1 5 5	95.31
1.027	1	5 2 4	97.15
1.027	2	4 0 5	97.17
1.027	3	1 8 3	97.23
1.010	2	2 5 5	99.45
1.001	1	6 5 0	100.69
.9985	3	5 5 3	100.97
.9882	1	6 5 1	102.43
.9874	1	2 2 6	102.55
.9620	1	2 3 6	106.41
.9596	2	7 0 2	106.79
.9540	1	0 10 0	107.69
.9493	1	3 8 3	108.47
.9492	1	7 3 1	108.48
.9433	1	1 8 4	109.50
.9268	1	0 7 5	112.44
.9240	1	3 9 2	112.95
.9213	1	5 5 4	113.47
.9189	1	2 8 4	113.92
.9084	1	4 9 0	115.99
.9025	1	5 3 5	117.20
.8921	2	2 5 6	119.41
.8802	1	1 2 7	122.13
.8781	1	0 6 6	122.62
.8749	3	5 8 2	123.39

Cobalt gadolinium, Co_2Gd

Structure
Cubic, Fd3m(227), Z=8, C15 type, isostructural with Cu_2Mg [Wernick and Geller, 1960].

Lattice constant: [ibid.]

$a = 7.255(5)\text{Å}$.

Density
(calculated) 9.571 g/cm^3

Thermal parameters
Overall isotropic B = 1.0

Scattering factors
Co^0 and Gd^0 [Thomas and Umeda, 1957], corrected for dispersion [Dauben and Templeton, 1955].

Scale factors (integrated intensities)
$\gamma = 0.372 \times 10^{-3}$
I/I_c (calculated = 8.83

References

Dauben, C. H. and Templeton, D. H. (1955). Acta Crystallogr. 8, 841.
Thomas, L.H. and Umeda, K. (1957). J. Chem. Phys. 26, 293.
Wernick, J.H. and Geller, S. (1960). Trans. AIME 218, 866.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
4.19	12	1	1	1	21.20
2.564	64	2	2	0	34.96
2.187	100	3	1	1	41.24
2.094	17	2	2	2	43.16
1.664	2	3	3	1	55.14
1.481	15	4	2	2	62.68
1.396	19	5	1	1 +	66.96
1.283	13	4	4	0	73.82
1.226	1	5	3	1	77.82
1.147	4	6	2	0	84.36
1.106	5	5	3	3	88.26
1.094	3	6	2	2	89.54
.970	5	6	4	2	105.22
.945	8	7	3	1 +	109.28
.907	2	8	0	0	116.30
.855	3	8	2	2 +	128.56
.838	5	7	5	1 +	133.70
.832	1	6	6	2	135.52

Calculated Pattern (Integrated)

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
4.19	10	1	1	1	21.19
2.565	63	2	2	0	34.95
2.187	100	3	1	1	41.24
2.094	17	2	2	2	43.16
1.664	2	3	3	1	55.14
1.481	18	4	2	2	62.68
1.396	19	5	1	1	66.97
1.396	6	3	3	3	66.97
1.283	18	4	4	0	73.83
1.226	1	5	3	1	77.83
1.147	7	6	2	0	84.37
1.106	8	5	3	3	88.25
1.094	4	6	2	2	89.54
.969	9	6	4	2	105.22
.945	10	7	3	1	109.28
.945	5	5	5	3	109.28
.907	3	8	0	0	116.29
.855	2	6	6	0	128.56
.855	4	8	2	2	128.56
.838	11	7	5	1	133.71
.838	2	5	5	5	133.71
.832	3	6	6	2	135.52
.796	1	7	5	3	150.61

Cobalt gadolinium, Co_7Gd_2

Structure
Hexagonal, $R\bar{3}m(166)$, Z = 6. The structure was determined by Bertaut et al. [1965].

Lattice constants: [Ostertag, 1967]

a = 5.023Å
c = 36.29

Density
(calculated) 9.135 g/cm^3

Thermal parameters
Isotropic [Bertaut et al., op. cit.]

Scattering factors
Co^0, Gd^0 [Cromer and Mann, 1968].

Scale factors (integrated intensities)
$\gamma = 0.302 \times 10^{-3}$
I/I_c (calculated) = 6.84

References

Bertaut, E. F., Lemaire, F. G. R., and Schweizer, J. (1965). C. R. Acad. Sci. 260, 3595.

Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.

Ostertag, W. (1967). J. Less-Common Metals, 13, 385.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
12.10	7	0 0 3	7.30
4.319	7	1 0 1	20.56
4.032	6	0 0 9	22.04
3.922	3	1 0 4	22.66
3.140	4	0 1 8	28.42
3.024	1	0 0 12	29.52
2.787	43	1 0 10	32.10
2.629	25	0 1 11	34.08
2.512	50	1 1 0	35.72
2.459	1	1 1 3	36.52
2.419	1	0 0 15	37.14
2.349	4	1 0 13	38.28
2.227	10	0 1 14	40.48
2.171	35	0 2 1	41.56
2.132	100	1 1 9	42.36
2.115	11	0 2 4	42.70
2.083	4	2 0 5	43.40
2.016	16	0 0 18	44.92
2.006	8	0 2 7	45.16
1.961	9	2 0 8	46.26
1.932	2	1 1 12	47.00
1.916	5	0 1 17	47.40
1.816	1	2 0 11	50.20
1.742	3	1 1 15	52.48
1.728	2	0 0 21	52.94
1.675	4	0 1 20	54.78
1.666	1	2 0 14	55.06
1.642	1	2 1 1	55.94
1.572	4	1 1 18	58.68
1.546	1	1 2 8	59.78
1.524	1	2 0 17	60.74
1.512	1	0 0 24	61.26
1.498	10	2 1 10	61.90
1.483	2	0 1 23	62.58
1.472	7	1 2 11	63.14
1.450	7	3 0 0	64.18
1.435	7	0 2 19	64.92
1.424	5	1 1 21	65.52
1.417	2	2 1 13	65.86
1.393	7	2 0 20	67.12
1.388	5	1 2 14	67.38
1.377	1	1 0 25	68.04
1.364	18	0 3 9+	68.74
1.303	2	1 2 17	72.50
1.295	4	1 1 24	72.98
1.277	2	2 0 23	74.18
1.256	15	2 2 0	75.68
1.244	1	3 0 15+	76.54
1.218	3	1 2 20	78.44
1.210	1	0 0 30	79.10
1.203	1	0 1 29	79.66
1.199	1	2 2 9	79.94
1.185	2	1 1 27	81.08
1.177	1	3 0 18+	81.74
1.175	2	2 0 26	81.96
1.145	4	1 3 10	84.58
1.138	1	1 2 23	85.16
1.133	3	3 1 11	85.66
1.113	1	0 2 28+	87.56
1.111	3	0 3 21+	87.82
1.094	2	3 1 14	89.54
1.090	3	1 1 30	89.96
1.087	4	4 0 1+	90.24
1.066	8	2 2 18	92.56
1.058	1	0 4 8	93.50
1.050	1	3 1 17	94.34
1.047	2	0 3 24+	94.78
1.037	1	1 0 34	96.00
1.031	1	0 2 31	96.70
1.016	2	2 2 21	98.62

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.007	2	1 1 33+	99.74
1.005	2	3 1 20	100.12
.9958	1	1 2 29	101.36
.9857	1	0 3 27+	102.78
.9660	1	2 2 24	105.76
.9622	3	3 2 10	106.36
.9582	2	0 2 34+	107.00
.9552	2	2 3 11	107.48
.9536	1	2 1 31	107.76
.9493	4	4 1 0	108.48
.9451	2	4 0 19	109.18
.9359	1	2 0 35+	110.78
.9328	2	0 4 20	111.34
.9313	2	2 3 14	111.60
.9289	3	3 0 30+	112.04
.9278	1	1 3 25	112.22
.9240	11	1 4 9+	112.96
.8953	2	2 1 34+	118.72
.8881	1	1 0 40	120.30
.8762	1	3 0 33+	123.08
.8744	2	2 3 20	123.52
.8726	2	1 1 39	124.00
.8712	2	2 2 30	124.30
.8686	2	3 1 29	124.96
.8588	1	1 4 18+	127.52
.8579	1	0 4 26	127.78
.8460	1	0 5 10	131.14
.8434	1	2 3 23	131.92
.8412	1	5 0 11	132.60
.8402	1	1 3 31	132.94
.8372	2	3 3 0+	133.88
.8320	2	4 1 21+	135.60
.8285	1	1 0 43	136.80
.8273	1	2 2 33	137.20
.8219	3	2 4 1	139.18
.8197	6	3 3 9	140.00
.8103	1	0 1 44	143.84
.8089	1	4 2 8	144.46
.8040	3	4 1 24+	146.72
.7994	1	1 3 34	148.98
.7977	1	4 2 11	150.00
.7968	1	4 0 31	150.38
.7943	1	2 1 40	151.74
.7861	4	2 2 36	156.98
.7831	1	0 3 39+	159.22

Calculated Pattern (Integrated)			
d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
12.10	5	0 0 3	7.30
4.319	6	1 0 1	20.55
4.032	5	0 0 9	22.03
3.922	3	1 0 4	22.65
3.140	4	0 1 8	28.40
3.024	1	0 0 12	29.51
2.787	40	1 0 10	32.09
2.629	24	0 1 11	34.08
2.512	48	1 1 0	35.72
2.459	1	1 1 3	36.51
2.419	1	0 0 15	37.13
2.349	4	1 0 13	38.29
2.227	10	0 1 14	40.48
2.171	33	0 2 1	41.56
2.160	7	2 0 2	41.79
2.132	100	1 1 9	42.36
2.115	5	0 2 4	42.72
2.083	3	2 0 5	43.40
2.016	16	0 0 18	44.92
2.006	5	0 2 7	45.17
1.961	9	2 0 8	46.25
1.932	2	1 1 12	46.99
1.916	5	0 1 17	47.40
1.816	1	2 0 11	50.20
1.742	3	1 1 15	52.47
1.728	2	0 0 21	52.94
1.675	5	0 1 20	54.77
1.666	1	2 0 14	55.07
1.642	1	2 1 1	55.94
1.572	4	1 1 18	58.67
1.570	1	0 2 16	58.77
1.546	1	1 2 8	59.78
1.524	1	2 0 17	60.74
1.512	1	0 0 24	61.25
1.498	11	2 1 10	61.91
1.483	1	0 1 23	62.57
1.472	7	1 2 11	63.13
1.450	8	3 0 0	64.18
1.435	7	0 2 19	64.92
1.424	6	1 1 21	65.51
1.417	1	2 1 13	65.89
1.393	7	2 0 20	67.13
1.398	4	1 2 14	67.39
1.377	1	1 0 25	68.03
1.364	10	3 0 9	68.74
1.364	10	0 3 9	68.74
1.303	2	1 2 17	72.51
1.295	4	1 1 24	72.97
1.277	2	2 0 23	74.19
1.256	17	2 2 0	75.67

Cobalt gadolinium, Co_7Gd_2 - continued

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.218	3	1 2 20	78.43
1.210	1	0 0 30	79.11
1.203	1	0 1 29	79.66
1.199	1	2 2 9	79.95
1.185	3	1 1 27	81.09
1.175	2	2 0 26	81.95
1.145	4	1 3 10	84.57
1.138	1	1 2 23	85.16
1.133	3	3 1 11	85.66
1.113	1	0 2 28	87.55
1.111	1	0 3 21	87.81
1.111	1	3 0 21	87.81
1.094	2	3 1 14	89.54
1.090	4	1 1 30	89.95
1.088	1	2 1 25	90.13
1.087	3	4 0 1	90.25
1.066	9	2 2 18	92.55
1.058	1	0 4 8	93.50
1.050	1	3 1 17	94.34
1.047	1	3 0 24	94.79
1.047	1	0 3 24	94.79
1.037	1	1 0 34	95.99
1.031	1	0 2 31	96.71
1.016	2	2 2 21	98.62
1.008	1	0 0 36	99.66
1.007	2	1 1 33	99.76
1.005	2	3 1 20	100.12
.9958	2	1 2 29	101.35
.9857	1	3 0 27	102.79
.9857	1	0 3 27	102.79
.9660	2	2 2 24	105.76
.9622	3	3 2 10	106.36
.9584	1	3 1 23	106.98
.9582	2	0 2 34	107.01
.9552	2	2 3 11	107.49
.9536	1	2 1 31	107.76
.9493	5	4 1 0	108.48
.9451	2	4 0 10	109.19
.9359	1	2 0 35	110.78
.9328	2	0 4 20	111.34
.9313	1	2 3 14	111.60
.9289	1	3 0 30	112.05
.9289	1	0 3 30	112.05
.9278	1	1 3 25	112.24
.9240	7	4 1 0	112.95
.9240	7	1 4 0	112.95
.9041	1	2 3 17	116.87
.8954	1	0 4 23	118.69
.8953	2	2 1 34	118.73
.8881	1	1 0 40	120.30
.8762	1	0 3 33	123.07
.8762	1	3 0 33	123.07
.8744	2	2 3 20	123.50
.8726	1	1 1 39	123.97
.8712	3	2 2 30	124.30
.8686	2	3 1 29	124.97
.8588	1	4 1 18	127.51
.8588	1	1 4 18	127.51
.8579	1	0 4 26	127.78
.8460	2	0 5 10	131.14
.8434	1	2 3 23	131.93
.8423	1	2 1 37	132.27
.8412	1	5 0 11	132.60
.8402	1	1 3 31	132.94
.8372	3	3 3 0	133.89
.8331	1	4 0 28	135.23
.8320	2	4 1 21	135.59
.8320	2	1 4 21	135.59
.8285	2	1 0 43	136.79
.8273	2	2 2 33	137.21
.8248	1	5 0 14	138.11
.8224	1	3 2 25	139.00
.8219	6	2 4 1	139.19
.8212	1	4 2 2	139.43
.8197	9	3 3 9	140.02
.8187	1	2 4 4	140.39
.8119	1	2 4 7	143.14
.8103	2	0 1 44	143.83
.8089	1	4 2 8	144.45
.8040	3	1 4 24	146.72
.8040	3	4 1 24	146.72
.7994	3	1 3 34	148.98
.7977	1	4 2 11	149.89
.7968	2	4 0 31	150.39
.7943	4	2 1 40	151.73
.7911	1	3 3 15	153.64
.7868	1	0 2 43	156.49
.7861	12	2 2 36	156.98
.7845	2	5 0 20	158.17
.7836	1	4 2 14	158.84
.7831	2	0 3 39	159.23
.7831	2	3 0 39	159.23

Cobalt gallium manganese, Co_2GaMn

Structure
Cubic, Fm3m(225), Z=4, Heusler alloy, type $L2_1$, from powder data (x-ray and neutron) [Webster, 1971].

Lattice constant: [ibid.]

$a = 5.770\text{Å}$

Density
(calculated) 8.383 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Ga^0, Mn^0 [Cromer and Mann, 1968].

Scale factors (integrated intensities)
$\gamma = 0.851 \times 10^{-3}$
I/I_c (calculated) = 12.4

References
Cromer, D. T. and Webster, J. B. (1968). Acta Crystallogr. A24, 321.
Webster, P.J. (1971). J. Phys. Chem. Solids, 32, 1221.

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.331	1	1 1 1	26.74
2.040	100	2 2 0	44.37
1.4425	13	4 0 0	64.55
1.1778	23	4 2 2	81.69
1.0200	7	4 4 0	98.08
.9123	11	6 2 0	115.20
.8328	4	4 4 4	135.31

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.331	1	1 1 1	26.74
2.040	100	2 2 0	44.38
1.4425	12	4 0 0	64.56
1.1778	20	4 2 2	81.70
1.0200	6	4 4 0	98.08
.9123	8	6 2 0	115.20
.8328	2	4 4 4	135.32

Cobalt gallium tantalum, Co_2GaTa

Structure
Cubic, Fm3m(225), Z=4, Heusler alloy, type $L2_1$, from powder data [Markiv et al., 1965].

Lattice constant: [ibid.]

$a = 5.923\text{Å}$

Density
(calculated) 11.780 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Ga^0, Ta^0 [Cromer and Mann, 1968].

Scale factors (integrated intensities)
$\gamma = 1.56 \times 10^{-3}$
I/I_c (calculated) = 18.7

References
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Markiv, V. Ya., Voroshilov, Yu.V., Kripyakevich, P.I., and Cherkashin, E. E. (1965). Sov. Phys. Crystallogr. 9, 619.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.420	24	1 1 1	26.04
2.961	18	2 0 0	30.16
2.094	100	2 2 0	43.16
1.786	10	3 1 1	51.10
1.710	4	2 2 2	53.56
1.481	13	4 0 0	62.70
1.359	3	3 3 1	69.06
1.324	5	4 2 0	71.12
1.209	22	4 2 2	79.16
1.140	2	5 1 1+	85.02
1.047	6	4 4 0	94.74
1.001	3	5 3 1	100.60
.9872	2	4 4 2+	102.58
.9365	10	6 2 0	110.68
.9032	1	5 3 3	117.04
.8929	2	6 2 2	119.24
.8549	3	4 4 4	128.58
.8294	2	7 1 1+	136.48
.8214	1	6 4 0	139.38
.7915	16	6 4 2	153.42

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.420	21	1 1 1	26.04
2.961	16	2 0 0	30.15
2.094	100	2 2 0	43.17
1.786	10	3 1 1	51.10
1.710	4	2 2 2	53.55
1.481	14	4 0 0	62.69
1.359	4	3 3 1	69.07
1.324	5	4 2 0	71.13
1.209	26	4 2 2	79.16
1.140	2	5 1 1	85.03
1.140	1	3 3 3	85.03
1.047	8	4 4 0	94.73
1.001	3	5 3 1	100.60
.9872	2	4 4 2	102.58
.9365	13	6 2 0	110.68
.9032	1	5 3 3	117.04
.8929	2	6 2 2	119.24
.8549	4	4 4 4	128.59
.8294	2	5 5 1	136.49
.8294	2	7 1 1	136.48
.8214	3	6 4 0	139.38
.7915	43	6 4 2	153.42

Cobalt gallium titanium, Co_2GaTi

Structure
Cubic, Fm3m, Z=4, Heusler alloy, type $L2_1$, from powder data (x-ray and neutron) [Webster and Ziebeck, 1973].

Lattice constant: [ibid.]

$a = 5.848\text{Å}$

Density
(calculated) 7.818 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Ga^0, Ti^0 [Cromer and Mann, 1968].

Scale factors (integrated intensities)
$\gamma = 0.885 \times 10^{-3}$
I/I_c (calculated) = 11.9

References
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Webster, P. J. and Ziebeck, K. R. A. (1973). J. Phys. Chem. Solids, 34, 1647.

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.376	3	1 1 1	26.38
2.068	100	2 2 0	43.75
1.7632	2	3 1 1	51.81
1.4620	13	4 0 0	63.59
1.1937	23	4 2 2	80.38
1.0338	7	4 4 0	96.34
.9246	11	6 2 0	112.83
.8441	4	4 4 4	131.73

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.376	3	1 1 1	26.38
2.068	100	2 2 0	43.76
1.7632	1	3 1 1	51.82
1.4620	12	4 0 0	63.60
1.1937	20	4 2 2	80.38
1.0338	6	4 4 0	96.34
.9246	8	6 2 0	112.84
.8441	2	4 4 4	131.72

Cobalt gallium vanadium, Co_2GaV

Structure
Cubic, Fm3m(225), Z=4, Heusler alloy, type $L2_1$, from powder data (x-ray and neutron) [Ziebeck and Webster, 1974].

Lattice constant: [ibid.]

$a = 5.786\text{Å}$

Density
(measured) 8.15 g/cm^3 [ibid.]
(calculated) 8.177 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Ga^0, V^0 [Cromer and Mann, 1968].

Scale factors (integrated intensities)
$\gamma = 0.893 \times 10^{-3}$
I/I_c (calculated) = 12.0

References
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Ziebeck, K. R. A. and Webster, P. J. (1974). J. Phys. Chem. Solids, 35, 1.

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.341	2	1 1 1	26.66
2.046	100	2 2 0	44.24
1.7445	1	3 1 1	52.41
1.4465	13	4 0 0	64.35
1.1811	23	4 2 2	81.42
1.0228	7	4 4 0	97.72
.9148	11	6 2 0	114.70
.8351	4	4 4 4	134.55

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.341	3	1 1 1	26.68
2.046	100	2 2 0	44.24
1.7445	1	3 1 1	52.40
1.4465	12	4 0 0	64.36
1.1811	20	4 2 2	81.42
1.0228	6	4 4 0	97.72
.9148	8	6 2 0	114.70
.8351	2	4 4 4	134.54

Cobalt germanium manganese, Co_2GeMn

Structure
Cubic, Fm3m(225), Z=4, Heusler alloy, type $L2_1$, from powder data (x-ray and neutron) [Webster, 1971].

Lattice constant: [ibid.]

$a = 5.743\text{Å}$

Density
(calculated) 8.594 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Ge^0, Mn^0 [Cromer and Mann, 1968].

Scale factors (integrated intensities)
$\gamma = 0.851 \times 10^{-3}$
I/I_c (calculated) = 12.4

References
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Webster, P.J. (1971). J. Phys. Chem. Solids, 32, 1221.

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.316	2	1 1 1	26.87
2.0305	100	2 2 0	44.59
1.7316	1	3 1 1	52.83
1.4357	13	4 0 0	64.89
1.1723	23	4 2 2	82.16
1.0152	7	4 4 0	98.71
.9080	12	6 2 0	116.05
.8289	4	4 4 4	136.64

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.316	2	1 1 1	26.88
2.0305	100	2 2 0	44.60
1.7316	1	3 1 1	52.82
1.4357	12	4 0 0	64.90
1.1723	20	4 2 2	82.16
1.0152	6	4 4 0	98.70
.9080	9	6 2 0	116.06
.8289	2	4 4 4	136.64

Cobalt germanium titanium, Co_2GeTi

Structure
Cubic, Fm3m(225), Z=4, Heusler alloy, type $L2_1$, from powder data (Gladyshevskii et al., 1963].

Lattice constant: [ibid.]

$a = 5.823\text{Å}$

Density
(calculated) 8.018 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Ge^0, Ti^0 [Cromer and Mann, 1968].

Scale factors (integrated intensities)
$\gamma = 0.884 \times 10^{-3}$
I/I_c (calculated) = 12.0

References
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Gladyshevskii, E. I., Markiv, V. Ya., Kuz'ma, Yu. B. and Cherkashin, E. E. (1963). Titan Ego Splavy, No. 10, 71.

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.362	3	1 1 1	26.49
2.059	100	2 2 0	43.94
1.756	2	3 1 1	52.05
1.456	13	4 0 0	63.90
1.189	23	4 2 2	80.79
1.029	7	4 4 0	96.89
.921	11	6 2 0	113.58
.840	4	4 4 4	132.84

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.362	4	1 1 1	26.50
2.059	100	2 2 0	43.94
1.756	2	3 1 1	52.04
1.456	12	4 0 0	63.90
1.189	20	4 2 2	80.80
1.029	6	4 4 0	96.90
.921	9	6 2 0	113.59
.840	2	4 4 4	132.84

Cobalt indium, $CoIn_3$

Structure
Tetragonal, P4/mbm(127), Z=2. The structure was determined by Stadelmaier et al. [1973].

Lattice constants: [ibid.]

$a = 6.830$ Å
$c = 3.547$

Density
(measured) 8.09 g/cm^3 [ibid.]
(calculated) 8.097 g/cm^3

Thermal parameters
Isotropic [Stadelmaier et al., op. cit.].

Scattering factors
Co^0, In^0 [Cromer and Mann, 1968].

Scale factors (integrated intensities)
$\gamma = 0.451 \times 10^{-3}$
I/I_c (calculated) = 7.04

References

Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Stadelmaier, H. H., Schöbel, J. D., Jones, R. A., and Shumaker, C. A. (1973). Acta Crystallogr. B29, 2926.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.830	2	1 1 0	18.36
3.547	2	0 0 1	25.10
3.054	39	2 1 0	29.22
2.859	53	1 1 1	31.26
2.460	38	2 0 1	36.50
2.415	13	2 2 0	37.20
2.315	100	2 1 1	38.88
2.160	59	3 1 0	41.80
1.996	5	2 2 1	45.40
1.773	15	0 0 2	51.48
1.707	2	4 0 0	53.64
1.671	3	3 2 1	54.90
1.657	3	4 1 0	55.42
1.610	3	3 3 0	57.18
1.539	12	4 0 1	60.10
1.534	12	2 1 2	60.28
1.527	9	4 2 0	60.58
1.501	9	4 1 1	61.76
1.466	13	3 3 1	63.40
1.429	3	2 2 2	65.22
1.403	1	4 2 1	66.62
1.371	19	3 1 2	68.38
1.339	1	5 1 0	70.22
1.268	2	5 2 0	74.80
1.253	3	5 1 1	75.86
1.230	1	4 0 2	77.54
1.211	2	4 1 2	79.04
1.207	4	4 4 0	79.28
1.194	11	5 2 1	80.34
1.192	7	3 3 2	80.56
1.171	1	5 3 0	82.24
1.157	4	4 2 2	83.46
1.148	2	1 1 3	84.24
1.138	4	6 0 0	85.18
1.117	2	2 0 3	87.18
1.112	1	5 3 1	87.66
1.103	5	2 1 3	88.64
1.070	1	6 1 1	92.04
1.069	1	5 1 2	92.22
1.067	1	5 4 0	92.48
1.033	3	6 2 1	96.42
1.032	2	5 2 2	96.60
1.021	3	5 4 1	97.90
.9981	3	4 4 2	101.04
.9774	1	5 3 2	104.02
.9720	2	4 0 3	104.84
.9623	2	4 1 3	106.34
.9580	5	6 0 2	107.04
.9529	2	3 3 3	107.86
.9320	3	7 1 1+	111.48
.9151	3	6 4 1	114.66
.9141	1	5 4 2	114.84
.9070	1	7 2 1	116.28
.8968	4	7 3 0	118.40
.8867	2	0 0 4+	120.64
.8648	4	5 2 3	125.92
.8516	1	2 1 4	129.52
.8491	1	6 5 1	130.24
.8472	1	8 1 0	130.84
.8324	1	2 2 4+	135.48
.8240	3	8 1 1	138.40
.8203	4	3 1 4	139.78
.8049	2	6 6 0	146.28
.8003	7	7 3 2	148.52
.7974	2	6 2 3	150.04
.7920	2	5 4 3	153.12

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
4.830	1	1	1	0	18.36
3.547	2	0	0	1	25.09
3.054	37	2	1	0	29.21
2.859	52	1	1	1	31.26
2.460	38	2	0	1	36.49
2.415	13	2	2	0	37.20
2.315	100	2	1	1	38.88
2.160	60	3	1	0	41.79
1.996	5	2	2	1	45.40
1.773	16	0	0	2	51.49
1.707	2	4	0	0	53.63
1.671	3	3	2	1	54.90
1.657	3	4	1	0	55.42
1.610	4	3	3	0	57.17
1.539	12	4	0	1	60.09
1.534	7	2	1	2	60.30
1.527	8	4	2	0	60.59
1.501	10	4	1	1	61.76
1.466	14	3	3	1	63.40
1.429	4	2	2	2	65.22
1.403	2	4	2	1	66.62
1.371	22	3	1	2	68.39
1.339	1	5	1	0	70.21
1.268	2	5	2	0	74.80
1.253	3	5	1	1	75.86
1.230	1	4	0	2	77.55
1.211	2	4	1	2	79.03
1.207	3	4	4	0	79.28
1.194	12	5	2	1	80.33
1.192	2	3	3	2	80.51
1.171	2	5	3	0	82.24
1.157	5	4	2	2	83.46
1.148	2	1	1	3	84.25
1.138	5	6	0	0	85.17
1.117	2	2	0	3	87.17
1.112	1	5	3	1	87.67
1.103	6	2	1	3	88.63
1.070	2	6	1	1	92.04
1.069	1	5	1	2	92.22
1.067	1	5	4	0	92.47
1.033	3	6	2	1	96.42
1.032	2	5	2	2	96.61
1.021	4	5	4	1	97.89
.9981	4	4	4	2	101.03
.9774	2	5	3	2	104.02
.9720	2	4	0	3	104.83
.9623	2	4	1	3	106.34
.9580	6	6	0	2	107.04
.9529	3	3	3	3	107.87
.9320	3	7	1	1	111.49
.9151	4	6	4	1	114.66
.9141	1	5	4	2	114.85
.9070	1	7	2	1	116.27
.8968	6	7	3	0	118.39
.8867	2	0	0	4	120.61
.8864	1	5	1	3	120.69
.8648	7	5	2	3	125.92
.8516	1	2	1	4	129.52
.8491	2	6	5	1	130.25
.8472	1	8	1	0	130.81
.8324	1	2	2	4	135.46
.8240	6	8	1	1	138.41
.8240	1	7	4	1	138.41
.8203	8	3	1	4	139.78
.8142	1	6	1	3	142.20
.8066	2	8	2	1	145.51
.8049	3	6	6	0	146.27
.8003	17	7	3	2	148.52
.7974	4	6	2	3	150.05
.7920	5	5	4	3	153.12
.7870	1	4	0	4	156.38

Cobalt lanthanum, $CoLa_3$

Structure
Orthorhombic, Pnma(62), Z=4, isostructural with CFe_3, type DO_{11}. The structure was determined by Cromer and Larson [1961].

Lattice constants: [ibid.]

a = 7.279Å
b = 10.089
c = 6.578
(published value b = 10.088)

Density
(measured) 6.48 g/cm^3 [ibid.]
(calculated) 6.539 g/cm^3

Thermal parameters
Isotropic (Cromer and Larson, op. cit.].

Scattering factors
Co^0, La^0 [Forsyth and Wells, 1959].

Scale factors (integrated intensities)
$\gamma = 0.200 \times 10^{-3}$
I/I_c (calculated) = 4.15

References
Cromer, D. T. and Larson, A. C. (1961). Acta Crystallogr. 14, 1226.
Forsyth, J.B. and Wells, M. (1959). Acta Crystallogr. 12, 412.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
5.51	1	0	1	1	16.08
4.88	2	1	0	1	18.18
4.39	1	1	1	1	20.20
3.508	15	1	2	1	25.38
3.424	14	2	1	0	26.02
3.289	10	0	0	2	27.10
3.185	14	2	0	1	28.00
3.037	31	2	1	1	29.40
2.994	100	0	3	1+	29.82
2.952	33	2	2	0	30.26
2.873	51	1	1	2	31.10
2.769	32	1	3	1	32.30
2.693	45	2	2	1	33.24
2.577	12	1	2	2	34.80
2.522	5	0	4	0	35.56
2.470	16	2	3	0	36.34
2.440	2	2	0	2	36.80
2.372	8	2	1	2	37.90
2.312	1	2	3	1	38.92
2.276	13	3	0	1	39.56
2.241	3	1	4	1+	40.26
2.221	6	3	1	1	40.60
2.197	3	2	2	2	41.06
2.073	4	2	4	0	43.62
2.055	3	1	1	3	44.02
1.977	5	2	4	1+	45.88
1.953	1	3	0	2	46.48
1.938	15	1	2	3	46.84
1.885	3	3	3	1	48.24
1.878	3	2	0	3	48.38
1.821	2	3	2	2+	50.06
1.781	14	1	3	3	51.26
1.765	6	2	5	0	51.76
1.760	5	2	2	3	51.90
1.754	11	4	0	1	52.10
1.728	2	4	1	1	52.94
1.712	1	4	2	0	53.50
1.704	7	2	5	1	53.74
1.689	15	3	3	2	54.28
1.681	11	0	6	0	54.52
1.674	12	1	5	2	54.80
1.645	2	0	0	4	55.86
1.640	2	2	3	3	56.02
1.627	9	3	0	3	56.52
1.614	4	1	4	3	57.02
1.604	8	1	0	4	57.40
1.600	12	4	3	0	57.54
1.584	1	1	1	4	58.18
1.555	4	2	5	2	59.38
1.548	2	3	2	3	59.66
1.544	2	3	4	2	59.84
1.529	1	1	2	4	60.52
1.518	1	4	2	2	60.96
1.510	1	3	5	1	61.34
1.506	1	2	4	3	61.50
1.4972	1	0	6	2	61.92
1.4869	1	2	6	1	62.40
1.4924	2	2	1	4	62.60
1.4665	3	1	6	2	63.38
1.4548	3	1	5	3	63.94
1.4478	1	1	3	4	64.28
1.4391	3	4	3	2+	64.72
1.4366	3	2	2	4	64.86
1.4075	1	5	1	1+	66.36
1.4032	2	3	5	2	66.58
1.3681	1	5	2	1	68.54
1.3525	3	3	6	1	69.44
1.3493	2	4	2	3+	69.62
1.3237	1	4	5	1	71.18
1.3143	1	3	2	4+	71.78

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
1.2989	1	1	7	2	72.74
1.2872	4	5	2	2	73.52
1.2618	5	3	3	4	75.24
1.2557	1	1	5	4	75.68
1.2528	1	2	6	3	75.90
1.2378	1	5	3	2+	76.98
1.2280	1	2	1	5	77.70
1.2252	4	0	3	5	77.92
1.2177	1	3	7	1	78.48
1.2138	4	4	6	1+	78.80
1.2082	1	1	3	5	79.22
1.2042	3	5	1	3+	79.54
1.2016	3	2	2	5	79.76
1.1916	1	2	8	0	80.54
1.1848	1	6	1	1+	81.10
1.1795	2	6	2	0+	81.56
1.1773	2	5	4	2+	81.74
1.1725	3	2	8	1	82.14
1.1692	4	3	6	3	82.42
1.1624	2	1	8	2+	83.04
1.1607	3	1	6	4+	83.16
1.1470	1	4	3	4	84.38
1.1412	1	6	3	0+	84.92
1.1382	1	6	0	2	85.18
1.1285	1	3	5	4	86.10
1.1273	1	3	2	5	86.20
1.1244	2	6	3	1	86.48
1.1051	1	0	9	1	88.38
1.0963	1	0	0	6	89.28
1.0896	1	1	5	5+	89.96
1.0811	2	1	8	3	90.88
1.0785	1	6	4	1+	91.16
1.0662	1	4	0	5+	92.54
1.0548	1	2	5	5	93.82
1.0441	1	2	1	6	95.08
1.0395	3	5	5	3+	95.64

Calculated Pattern (Integrated)

d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
5.51	1	0	1	1	16.07
5.04	1	0	2	0	17.57
4.88	2	1	0	1	18.16
4.39	1	1	1	1	20.20
3.508	20	1	2	1	25.37
3.424	18	2	1	0	26.01
3.289	13	0	0	2	27.09
3.185	19	2	0	1	28.00
3.037	41	2	1	1	29.39
2.997	43	1	0	2	29.78
2.994	100	0	3	1	29.81
2.952	43	2	2	0	30.26
2.873	72	1	1	2	31.10
2.769	44	1	3	1	32.30
2.755	10	0	2	2	32.47
2.693	66	2	2	1	33.24
2.577	17	1	2	2	34.79
2.522	7	0	4	0	35.56
2.470	23	2	3	0	36.34
2.440	2	2	0	2	36.80
2.372	12	2	1	2	37.90
2.312	1	2	3	1	38.92
2.276	19	3	0	1	39.56
2.241	2	1	4	1	40.21
2.238	2	1	3	2	40.27
2.221	9	3	1	1	40.59
2.197	4	2	2	2	41.06
2.073	6	2	4	0	43.63
2.055	4	1	1	3	44.02
1.977	6	2	4	1	45.86
1.975	2	2	3	2	45.91
1.953	1	3	0	2	46.47
1.938	23	1	2	3	46.83
1.929	3	0	5	1	47.07
1.885	4	3	3	1	48.24
1.878	2	2	0	3	48.43
1.821	2	3	2	2	50.05
1.820	1	4	0	0	50.09
1.781	21	1	3	3	51.26
1.765	8	2	5	0	51.76
1.760	1	2	2	3	51.91
1.754	16	4	0	1	52.11
1.728	4	4	1	1	52.95
1.712	1	4	2	0	53.49
1.704	11	2	5	1	53.74
1.690	1	3	4	1	54.24
1.689	22	3	3	2	54.28
1.681	12	0	6	0	54.53
1.674	17	1	5	2	54.80
1.645	3	0	0	4	55.86

Cobalt lanthanum, $CoLa_3$ - continued

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.640	1	2 3 3	56.04
1.627	14	3 0 3	56.52
1.614	6	1 4 3	57.03
1.606	2	3 1 3	57.32
1.604	9	1 0 4	57.40
1.600	14	4 3 0	57.54
1.584	1	1 1 4	58.19
1.555	6	2 5 2	59.39
1.548	2	3 2 3	59.67
1.544	1	3 4 2	59.86
1.529	2	1 2 4	60.52
1.518	2	4 2 2	60.97
1.510	2	3 5 1	61.35
1.506	1	2 4 3	61.51
1.4972	1	0 6 2	61.93
1.4869	2	2 6 1	62.40
1.4824	2	2 1 4	62.62
1.4665	5	1 6 2	63.37
1.4548	5	1 5 3	63.94
1.4478	2	1 3 4	64.29
1.4391	4	4 3 2	64.72
1.4366	3	2 2 4	64.85
1.4079	1	0 7 1	66.34
1.4075	1	5 1 1	66.36
1.4032	2	3 5 2	66.59
1.3681	1	5 2 1	68.53
1.3525	4	3 6 1	69.43
1.3493	1	4 2 3	69.62
1.3237	2	4 5 1	71.17
1.3143	1	3 2 4	71.76
1.2989	2	1 7 2	72.75
1.2884	1	2 4 4	73.44
1.2872	7	5 2 2	73.52
1.2618	8	3 3 4	75.25
1.2557	1	1 5 4	75.68
1.2528	1	2 6 3	75.89
1.2378	1	5 3 2	76.97
1.2372	1	2 0 5	77.01
1.2280	2	2 1 5	77.70
1.2252	5	0 3 5	77.91
1.2210	1	1 8 1	78.23
1.2177	1	3 7 1	78.48
1.2138	6	4 6 1	78.78
1.2132	1	6 0 0	78.83
1.2128	1	5 0 3	78.86
1.2082	1	1 3 5	79.22
1.2045	1	6 1 0	79.51
1.2042	4	5 1 3	79.54
1.2031	1	2 5 4	79.62
1.2016	1	2 2 5	79.74

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
1.1916	2	2 8 0	80.55
1.1848	1	6 1 1	81.11
1.1795	1	6 2 0	81.54
1.1775	1	0 8 2	81.71
1.1773	2	5 4 2	81.73
1.1757	1	0 6 4	81.87
1.1725	5	2 8 1	82.14
1.1692	6	3 6 3	82.42
1.1624	2	1 8 2	83.01
1.1620	1	5 5 1	83.04
1.1607	3	1 6 4	83.16
1.1470	2	4 3 4	84.38
1.1412	1	6 3 0	84.91
1.1382	1	6 0 2	85.18
1.1285	1	3 5 4	86.09
1.1273	1	3 2 5	86.21
1.1244	3	6 3 1	86.48
1.1051	2	0 9 1	88.38
1.0963	1	0 0 6	89.27
1.0925	1	1 9 1	89.67
1.0900	1	5 0 4	89.93
1.0896	1	1 5 5	89.97
1.0811	3	1 8 3	90.88
1.0662	2	4 0 5	92.52
1.0655	1	5 2 4	92.60
1.0548	2	2 5 5	93.82
1.0441	1	2 1 6	95.08
1.0397	1	6 5 0	95.61
1.0395	4	5 5 3	95.64

Cobalt lutetium, Co_2Lu

Structure
Cubic, Fd3m(227), Z=8, isostructural with Cu_2Mg, type C15, from powder data [Lemaire, 1971].

Lattice constant: [ibid.]

$a = 7.102\text{Å}$

Density
(calculated) 10.860 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Lu^0 [Cromer and Mann, 1968].

Scale factors (integrated intensities)
$\gamma = 1.08 \times 10^{-3}$
I/I_c (calculated) = 14.5

References

Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Lemaire, F. G. R. (1971). Solid State Commun. 9, 341.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.100	24	1 1 1	21.66
2.511	77	2 2 0	35.7[illegible]
2.141	100	3 1 1	42.1[illegible]
2.050	13	2 2 2	44.14
1.775	1	4 0 0	51.4[illegible]
1.629	5	3 3 1	56.4[illegible]
1.450	21	4 2 2	64.20
1.367	23	5 1 1+	68.60
1.255	16	4 4 0	75.70
1.200	3	5 3 1	79.84
1.123	8	6 2 0	86.6[illegible]
1.083	7	5 3 3	90.6[illegible]
1.071	2	6 2 2	92.0[illegible]
.9945	2	7 1 1+	101.54
.9490	10	6 4 2	108.5[illegible]
.9246	14	7 3 1+	112.84
.8877	3	8 0 0	120.3[illegible]
.8676	1	7 3 3	125.20
.8370	6	8 2 2+	133.9[illegible]
.8201	8	7 5 1+	139.8[illegible]
.8147	1	6 6 2	142.0[illegible]
.7940	1	8 4 0	151.9[illegible]

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.100	20	1 1 1	21.66
2.511	73	2 2 0	35.7[illegible]
2.141	100	3 1 1	42.1[illegible]
2.050	12	2 2 2	44.14
1.775	1	4 0 0	51.4[illegible]
1.629	5	3 3 1	56.4[illegible]
1.450	23	4 2 2	64.1[illegible]
1.367	20	5 1 1	68.61
1.367	7	3 3 3	68.61
1.255	18	4 4 0	75.6[illegible]
1.200	4	5 3 1	79.8[illegible]
1.123	9	6 2 0	86.6[illegible]
1.083	8	5 3 3	90.67
1.071	3	6 2 2	92.02
.9945	1	5 5 1	101.5[illegible]
.9945	1	7 1 1	101.5[illegible]
.9490	12	6 4 2	108.5[illegible]
.9246	6	5 5 3	112.84
.9246	12	7 3 1	112.84
.8877	4	8 0 0	120.3[illegible]
.8676	1	7 3 3	125.20
.8370	7	8 2 2	133.95
.8370	3	6 6 0	133.95
.8201	15	7 5 1	139.87
.8201	2	5 5 5	139.87
.8147	2	6 6 2	142.01
.7940	2	8 4 0	151.9[illegible]

Cobalt neodymium, Co_2Nd

Structure
Cubic, Fd3m (227), Z = 8, isostructural with Cu_2Mg, type C15, from powder data [Harris et al., 1965].

Lattice constant: [ibid.]

a = 7.2986Å
(published value 7.2834 kX)

Density
(calculated) 8.955 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Nd^0 [Cromer and Mann, 1968].

Scale factors (integrated intensities)
$\gamma = 0.571 \times 10^{-3}$
I/I_c (calculated) = 12.2

References
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Harris, I. R., Mansey, R. C., and Raynor, G. V. (1965). J. Less-Common Metals, 9, 270.

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.214	11	1 1 1	21.07
2.5804	63	2 2 0	34.74
2.2006	100	3 1 1	40.98
2.1069	17	2 2 2	42.89
1.6744	2	3 3 1	54.78
1.4898	19	4 2 2	62.27
1.4046	19	5 1 1	66.52
1.4046	6	3 3 3	66.52
1.2902	18	4 4 0	73.31
1.2337	2	5 3 1	77.27
1.1540	7	6 2 0	83.75
1.1130	8	5 3 3	87.59
1.1003	4	6 2 2	88.87
.9753	10	6 4 2	104.33
.9502	11	7 3 1	108.32
.9502	5	5 5 3	108.32
.9123	3	8 0 0	115.20
.8601	2	6 6 0	127.16
.8601	5	8 2 2	127.16
.8428	12	7 5 1	132.13
.8428	2	5 5 5	132.13
.8372	3	6 6 2	133.88
.8011	2	7 5 3	148.11
.8011	1	9 1 1	148.11
.7780	13	6 6 4	163.83

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
4.214	12	1 1 1	21.08
2.5804	65	2 2 0	34.74
2.2006	100	3 1 1	40.98
2.1069	16	2 2 2	42.90
1.6744	2	3 3 1	54.78
1.4898	17	4 2 2	62.26
1.4046	23	5 1 1+	66.52
1.2902	16	4 4 0	73.32
1.2337	2	5 3 1	77.28
1.1540	6	6 2 0	83.74
1.1130	6	5 3 3	87.58
1.1003	3	6 2 2	88.86
1.0220	1	7 1 1+	97.82
.9753	7	6 4 2	104.34
.9502	12	7 3 1+	108.32
.9123	2	8 0 0	115.20
.8601	4	8 2 2+	127.16
.8428	7	7 5 1+	132.14
.8372	1	6 6 2	133.88
.8011	1	7 5 3+	148.10
.7780	3	6 6 4	163.82

Cobalt nickel tin, $Co_{.75}Ni_{.75}Sn_{.75}$

Structure
Hexagonal, $P6_3/mmc$ (194), Z=2, from powder data. The atoms were assigned these positions: 1.5 Co plus 0.5 Ni in 2a; 1.5 Sn plus 0.5 Ni in 2c; and only 0.5 Ni in 2d. [Castelliz, 1953].

Lattice constants: [ibid.]

a = 4.095Å
c = 5.209

Density
(calculated) 7.781 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
Co^0, Ni^0, Sn^0 [Cromer and Mann, 1968].

Scale factors (integrated intensities)
$\gamma = 0.453 \times 10^{-3}$
I/I_c (calculated) = 6.08

References
Castelliz, L. (1953). Monatsh. Chem. 84, 49.
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
2.931	100	1 0 1	30.48
2.604	7	0 0 2	34.42
2.099	87	1 0 2	43.06
2.048	88	1 1 0	44.20
1.679	14	2 0 1	54.64
1.610	7	1 1 2	57.18
1.559	11	1 0 3	59.20
1.466	20	2 0 2	63.40
1.302	5	0 0 4	72.54
1.298	11	2 1 1	72.80
1.241	4	2 0 3	76.76
1.192	16	2 1 2	80.52
1.182	9	3 0 0	81.32
1.099	14	1 1 4	89.02
1.076	2	3 0 2	91.38
1.061	5	2 1 3	93.10
1.024	5	2 2 0	97.60
1.000	2	1 0 5	100.82
.967	3	3 1 1	105.68
.953	1	2 2 2	107.90
.920	7	3 1 2	113.68
.898	2	2 0 5	118.08
.875	7	3 0 4	123.30
.874	2	4 0 1	123.60
.856	3	3 1 3	128.34
.843	3	1 0 6	131.98
.839	3	4 0 2	133.22
.823	3	2 1 5	138.94
.805	7	2 2 4	146.32
.804	3	3 2 1	146.78
.799	1	1 1 6	149.04
.790	1	4 0 3	154.60

Cobalt nickel tin, $Co_{.75}Ni_{.75}Sn_{.75}$ - continued

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
2.931	100	1	0	1	30.47
2.604	7	0	0	2	34.41
2.099	93	1	0	2	43.06
2.048	95	1	1	0	44.20
1.679	17	2	0	1	54.63
1.610	9	1	1	2	57.18
1.559	13	1	0	3	59.20
1.466	24	2	0	2	63.41
1.302	6	0	0	4	72.53
1.298	12	2	1	1	72.80
1.241	5	2	0	3	76.77
1.192	21	2	1	2	80.53
1.182	11	3	0	0	81.33
1.099	17	1	1	4	89.02
1.076	2	3	0	2	91.38
1.061	6	2	1	3	93.10
1.024	7	2	2	0	97.60
1.000	3	1	0	5	100.82
.967	5	3	1	1	105.69
.953	2	2	2	2	107.89
.920	10	3	1	2	113.68
.898	2	2	0	5	118.09
.875	12	3	0	4	123.30
.874	2	4	0	1	123.61
.856	5	3	1	3	128.34
.843	6	1	0	6	131.98
.839	6	4	0	2	133.21
.823	6	2	1	5	138.93
.805	17	2	2	4	146.31
.804	7	3	2	1	146.78
.799	2	1	1	6	149.05
.790	4	4	0	3	154.60

Cobalt samarium, Co_5Sm

Structure
Hexagonal, P6/mmm(191), Z=1, isostructural with $CaCu_5$, type $D2_d$, from powder data [Khan and Feldmann, 1973].

Lattice constants: [ibid.]

$a = 4.997 Å$
$c = 3.978$

Density
(measured) 8.58 g/cm^3 [ibid.]
(calculated) 8.590 g/cm^3

Thermal parameters
Isotropic: overall B = 2.0

Scattering factors
Co^0, Sm^0 [Cromer and Mann, 1968].

Scale factors (integrated intensities)
$\gamma = 0.320 \times 10^{-3}$
I/I_c (calculated) = 6.73

References
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Khan, Y. and Feldmann, D. (1973). J. Less-Common Metals, 31, 111.

Calculated Pattern (Peak heights)					
d(Å)	I	h	k	ℓ	2θ(°) λ = 1.540598Å
4.328	2	1	0	0	20.52
3.978	8	0	0	1	22.34
2.929	60	1	0	1	30.50
2.498	36	1	1	0	35.92
2.164	36	2	0	0	41.72
2.116	100	1	1	1	42.70
1.989	24	0	0	2	45.58
1.901	5	2	0	1	47.82
1.556	11	1	1	2	59.34
1.513	10	2	1	1	61.22
1.464	14	2	0	2	63.48
1.443	4	3	0	0	64.56
1.356	14	3	0	1	69.22
1.268	2	1	0	3	74.84
1.249	9	2	2	0	76.14
1.171	7	1	1	3	82.24
1.168	6	3	0	2	82.52
1.149	3	3	1	1	84.20
1.082	2	4	0	0	90.80
1.058	8	2	2	2	93.46
1.030	2	2	1	3	96.80
.994	1	0	0	4	101.54
.976	3	3	0	3	104.20
.963	1	3	2	1	106.20
.950	2	4	0	2	108.30
.944	1	4	1	0	109.32
.924	1	1	1	4	112.96
.919	5	4	1	1	113.94
.904	2	2	0	4	116.96
.890	1	3	1	3	119.92
.853	2	4	1	2	129.10
.819	1	3	0	4	140.38
.818	1	4	2	0	140.74
.815	2	3	3	1	141.80
.795	1	3	2	3	151.52

Cobalt samarium, Co_5Sm - continued

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
4.328	2	1	0	0	20.51
3.978	7	0	0	1	22.33
2.929	56	1	0	1	30.50
2.498	35	1	1	0	35.91
2.164	36	2	0	0	41.71
2.116	100	1	1	1	42.70
1.989	25	0	0	2	45.57
1.901	5	2	0	1	47.81
1.556	12	1	1	2	59.34
1.513	11	2	1	1	61.22
1.464	15	2	0	2	63.48
1.443	4	3	0	0	64.55
1.356	16	3	0	1	69.23
1.268	3	1	0	3	74.83
1.249	10	2	2	0	76.14
1.192	1	2	2	1	80.53
1.171	8	1	1	3	82.24
1.168	3	3	0	2	82.55
1.149	3	3	1	1	84.19
1.082	2	4	0	0	90.80
1.058	10	2	2	2	93.46
1.030	2	2	1	3	96.81
.994	1	0	0	4	101.53
.976	4	3	0	3	104.20
.963	2	3	2	1	106.20
.950	3	4	0	2	108.29
.944	2	4	1	0	109.31
.924	2	1	1	4	112.95
.919	7	4	1	1	113.94
.904	2	2	0	4	116.96
.890	2	3	1	3	119.92
.853	3	4	1	2	129.10
.846	1	5	0	1	131.24
.833	1	3	3	0	135.31
.819	2	3	0	4	140.37
.818	3	4	2	0	140.74
.815	4	3	3	1	141.81
.795	2	3	2	3	151.51
.782	2	1	0	5	159.75

Cobalt tin, Co_3Sn_2

Structure
Hexagonal, $P6_3/mmc$ (194), Z = 1, isostructural with Ni_3Sn_2, type $B8_2$, from powder data [Rajeswari and Manohar, 1970].

Lattice constants: [ibid.]

a = 4.109Å
c = 5.180

Density
(calculated) 9.080 g/cm^3

Thermal parameters
Isotropic: overall B = 1.0

Polymorphism
This phase was annealed above 550 °C, and quenched to room temperature. A low-temperature, more ordered modification also exists [Rajeswari and Manohar, op. cit.].

Scattering factors
Co^0, Sn^0 [Cromer and Mann, 1968].

Scale factors (integrated intensities)
$\gamma = 0.383 \times 10^{-3}$
I/I_c (calculated) = 6.62

References
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Rajeswari, H. and Manohar, H. (1970). Indian J. Pure Appl. Phys. 8, 363.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ = 1.540598Å
3.558	2	1 0 0	25.02
2.933	82	1 0 1	30.46
2.590	12	0 0 2	34.60
2.094	88	1 0 2	43.16
2.055	100	1 1 0	44.04
1.683	12	2 0 1	54.48
1.610	14	1 1 2	57.18
1.553	9	1 0 3	59.46
1.467	21	2 0 2	63.38
1.302	9	2 1 1	72.56
1.295	6	0 0 4	73.00
1.239	4	2 0 3	76.88
1.194	18	2 1 2	80.38
1.186	11	3 0 0	81.00
1.096	15	1 1 4	89.36
1.078	3	3 0 2	91.16
1.061	4	2 1 3	93.10
1.027	6	2 2 0	97.16
.995	2	1 0 5	101.50
.970	3	3 1 1	105.22
.955	2	2 2 2	107.54
.922	7	3 1 2	113.28
.895	1	2 0 5	118.72
.877	2	4 0 1	122.94
.875	9	3 0 4	123.44
.857	3	3 1 3	128.06
.841	3	4 0 2	132.56
.839	4	1 0 6	133.28
.821	2	2 1 5	139.62
.806	3	3 2 1	145.58
.805	8	2 2 4	146.34
.796	2	1 1 6	150.84
.791	1	4 0 3	153.84

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ = 1.540598Å
3.558	2	1	0	0	25.00
2.933	76	1	0	1	30.45
2.590	12	0	0	2	34.60
2.094	89	1	0	2	43.17
2.055	100	1	1	0	44.04
1.683	13	2	0	1	54.49
1.610	15	1	1	2	57.18
1.553	10	1	0	3	59.45
1.467	24	2	0	2	63.37
1.302	10	2	1	1	72.56
1.295	6	0	0	4	73.00
1.239	4	2	0	3	76.87
1.194	20	2	1	2	80.38
1.186	12	3	0	0	80.99
1.096	18	1	1	4	89.36
1.078	3	3	0	2	91.17
1.061	5	2	1	3	93.10
1.027	7	2	2	0	97.16
.995	2	1	0	5	101.50
.970	4	3	1	1	105.22
.955	3	2	2	2	107.55
.922	10	3	1	2	113.29
.895	2	2	0	5	118.72
.877	2	4	0	1	122.94
.875	13	3	0	4	123.44
.857	4	3	1	3	128.05
.841	5	4	0	2	132.56
.839	6	1	0	6	133.31
.821	5	2	1	5	139.61
.806	6	3	2	1	145.57
.805	18	2	2	4	146.33
.796	4	1	1	6	150.85
.791	4	4	0	3	153.83

Further work on this program is in progress, and it is anticipated that additional sections will be issued. Therefore, the accumulative index here is not necessarily the concluding index for the project.

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*Natural mineral.

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16. ABSTRACT (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here.)

Standard x-ray diffraction patterns are presented for 58 substances. Thirty-one of these patterns represent experimental data and 27 are calculated. The experimental x-ray powder diffraction patterns were obtained with an x-ray diffractometer. All d-values were assigned Miller indices determined by comparison with computed interplanar spacings consistent with space group extinctions. The densities and lattice constants were calculated, and the refractive indices were measured whenever possible. The calculated x-ray powder diffraction patterns were computed from published crystal structure data. Both peak height and integrated intensities are reported for the calculated patterns.

17. KEY WORDS (six to twelve entries; alphabetical order; capitalize only the first letter of the first key word unless a proper name; separated by semicolons)

Crystal structure; integrated intensities; lattice constants; peak intensities; powder patterns; reference intensities; standard; x-ray diffraction.

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